

(19) World Intellectual Property Organization
International Bureau



(43) International Publication Date
21 March 2002 (21.03.2002)

PCT

(10) International Publication Number
WO 02/22793 A1

(51) International Patent Classification⁷: C12N 9/00,
G06F 17/50

(21) International Application Number: PCT/GB01/04067

(22) International Filing Date:
11 September 2001 (11.09.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
09/659,759 11 September 2000 (11.09.2000) US

(63) Related by continuation (CON) or continuation-in-part
(CIP) to earlier application:
US 09/659,759 (CIP)
Filed on 11 September 2000 (11.09.2000)

(71) Applicant (for all designated States except US): **ASTEX
TECHNOLOGY LIMITED** [GB/GB]; 250 Cambridge
Science Park, Milton Road, Cambridge, Cambridgeshire
CB4 0WE (GB).

(72) Inventors; and

(75) Inventors/Applicants (for US only): **BLUNDELL, Tom,**
L. [GB/GB]; Rushmore House, Fowlmere Road, Shep-
peth, Royston, Hertfordshire SG8 6QP (GB). **ABELL,**
Christopher [GB/GB]; 39 Leys Avenue, Cambridge,
Cambridgeshire CB4 2AN (GB). **VON DELFT, Frank**
[ZA/US]; Scripps Research Institute, 10550 North Torrey
Pines Road, La Jolla, CA 92037 (US).

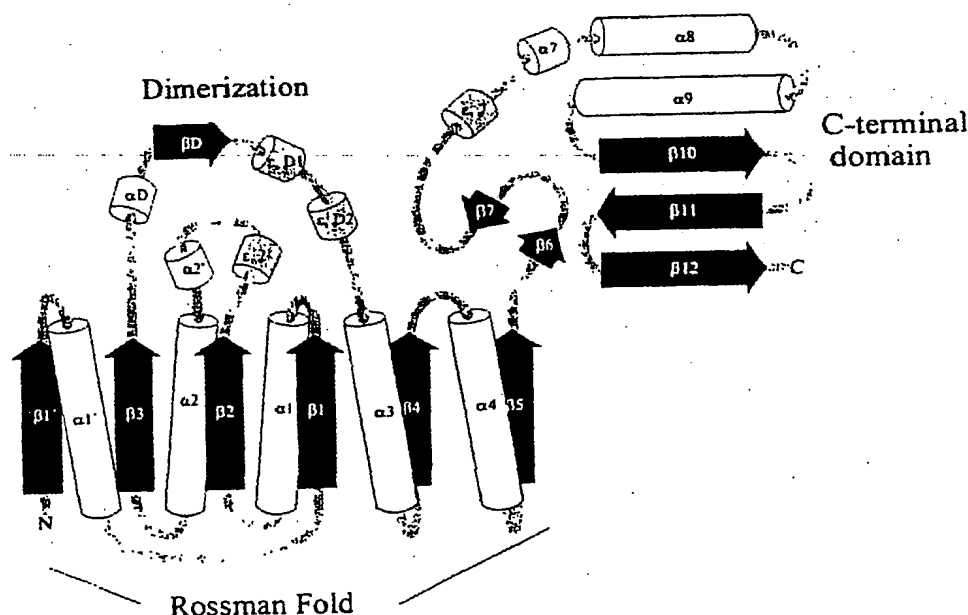
(74) Agents: **ARMITAGE, Ian, M.** et al.; Mewburn Ellis, York
House, 23 Kingsway, London, Greater London WC2B 6HP
(GB).

(81) Designated States (national): AE, AG, AL, AM, AT, AU,
AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU,
CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,
MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI,
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,
ZA, ZW.

(84) Designated States (regional): ARIPO patent (GH, GM,
KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian
patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European

[Continued on next page]

(54) Title: CRYSTAL STRUCTURE OF PANTOTHENATE SYNTHETASE



(57) Abstract: A crystal of pantothenate synthetase (PS) has a monoclinic space group $P2_1$ and unit cell dimensions of $a = 66.0 \pm 0.2 \text{ \AA}$, $b = 78.1 \pm 0.2 \text{ \AA}$, $c = 77.1 \pm 0.2 \text{ \AA}$ and $\beta = 103.7 \pm 0.2^\circ$.



patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

— entirely in electronic form (except for this front page) and available upon request from the International Bureau

Published:

- with international search report
- before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

CRYSTAL STRUCTURE OF PANTOTHENATE SYNTHETASE

Field of the Invention

5 The present invention relates to the enzyme pantothenate synthetase, and in particular its crystal structure and the use of this structure in drug discovery.

Background of the Invention

10

Pantothenic acid (vitamin B₅) is found in coenzyme A (CoA) and the acyl carrier protein (ACP), both of which are involved in fatty acid metabolism.

15

Pantothenic acid can be synthesised by plants and microorganisms but animals are apparently unable to make the vitamin, and require it in their diet. However, all organisms are able to convert pantothenic acid to its metabolically active form, coenzyme A.

20

The pathway for the synthesis of pantothenic acid is shown in Fig. 1. It provides a potential target for the treatment of infectious disease, since inhibitors of the pathway should be damaging to bacteria and fungi but not to human or animal subjects infected by bacteria.

25

Of specific interest is pantothenate synthetase (D-pantoate: β -alanine ligase (AMP-forming); EC 6.3.2.1). This enzyme catalyses the condensation between β -alanine and pantoic acid, the final steps in pantothenic acid biosynthesis. Inhibitors (whether competitive, non-competitive, uncompetitive or irreversible) of pantothenate synthetase would be of significant technical and commercial interest.

30

-2-

Purification of pantothenate synthetase (PS) to homogeneity was achieved by Miyatake et. al, (*J. Biochem.*, 79, (1976), 673-678). The enzyme was reported to require stoichiometric amounts of ATP as an energy source which is hydrolysed to AMP and inorganic pyrophosphate. The mechanism of the enzymic reaction involves pantoate adenylate as an intermediate.

However, until now no one has successfully determined the structure of PS. This has prevented PS inhibitors being developed via structure-based drug design methodologies. Knowledge of the structure of PS would significantly assist the rational design of novel therapeutics based on PS inhibitors.

Summary of the Invention

The present invention is at least partly based on overcoming several technical hurdles: we have (i) produced PS crystals of suitable quality, including crystals of selenium atom PS derivatives, for performing X-ray diffraction analyses, (ii) collected X-ray diffraction data from the crystals, (iii) determined a high resolution three-dimensional X-ray crystal structure of PS (i.e. a structure having a resolution which is numerically lower than 2 Å), and (iv) identified sites on the enzyme which are likely to be involved in the enzymic reaction.

In general aspects, the present invention is concerned with identifying or obtaining agent compounds (especially inhibitors of PS) for modulating PS activity, and in preferred embodiments identifying or obtaining actual agent compounds/inhibitors. Crystal structure information presented herein is useful in designing potential inhibitors and modelling them or their potential interaction with the PS

-3-

binding cavity. Potential inhibitors may be brought into contact with PS to test for ability to interact with the PS binding cavity. Actual inhibitors may be identified from among potential inhibitors synthesized following design and model work performed *in silico*. An inhibitor identified using the present invention may be formulated into a composition, for instance a composition comprising a pharmaceutically acceptable excipient, and may be used in the manufacture of a medicament for use in a method of treatment. These and other aspects and embodiments of the present invention are discussed below.

In a first aspect, the present invention provides a crystal of PS having a monoclinic space group $P2_1$, and unit cell dimensions of $a = 66.0 \pm 0.2 \text{ \AA}$, $b = 78.1 \pm 0.2 \text{ \AA}$, $c = 77.1 \pm 0.2 \text{ \AA}$ and $\beta = 103.7 \pm 0.2^\circ$. Preferably the PS is a dimer.

In a further aspect, the invention also provides a crystal of PS having the three dimensional atomic coordinates of Table 1. An advantageous feature of the structure defined by the atomic coordinates is that it has a high resolution, of about 1.7 \AA .

The coordinates of Table 1 provide a measure of atomic location in Angstroms, to a third decimal place. The coordinates are a relative set of positions that define a shape in three dimensions, but the skilled person would understand that an entirely different set of coordinates having a different origin and/or axes could define a similar or identical shape. Furthermore, the skilled person would understand that varying the relative atomic positions of the atoms of the structure so that the root mean square deviation of the residue backbone atoms (i.e. the nitrogen-carbon-carbon backbone atoms of the protein amino acid residues) is less than 1.5 \AA (preferably less than 1.0 \AA and more preferably

-4-

less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for the residue backbone atoms, will generally result in a structure which is substantially the same as the structure of Table 1 in terms of both its structural characteristics and potency for structure-based design of PS inhibitors. Likewise the skilled person would understand that changing the number and/or positions of the water molecules and/or substrate molecules of Table 1 will not generally affect the potency of the structure for structure-based design of PS inhibitors. Thus for the purposes described herein as being aspects of the present invention, it is within the scope of the invention if: the Table 1 coordinates are transposed to a different origin and/or axes; the relative atomic positions of the atoms of the structure are varied so that the root mean square deviation of residue backbone atoms is less than 1.5 Å (preferably less than 1.0 Å and more preferably less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for the residue backbone atoms; and/or the number and/or positions of water molecules and/or substrate molecules is varied. Reference herein to the coordinate data of Table 1 thus includes the coordinate data in which one or more individual values of the Table are varied in this way. By "root mean square deviation" we mean the square root of the arithmetic mean of the squares of the deviations from the mean.

Thus, for example, varying the atomic positions of the atoms of the structure by up to about 0.2 Å in any direction will result in a structure which is substantially the same as the structure of Table 1 in terms of both its structural characteristics and utility e.g. for structure-based drug design.

The provision of the high resolution structure of Table 1

-5-

provides those of skill in the art with a detailed insight into the mechanisms of action of PS. This insight provides a means to design new antibacterial agents which have the potential to inhibit the process of pantothenate synthesis in bacteria and fungi, or to modulate the activity of the enzyme, for example such that the enzyme works more effectively on prodrugs which are converted by PS into an antibacterial drug.

In a further aspect, the invention provides a method for crystallizing a selenium atom PS derivative which comprises producing PS by recombinant production in a bacterial host (e.g. *E.coli*) in the presence of selenomethionine, recovering a selenium atom PS derivative from the host and growing crystals from the recovered selenium atom PS derivative.

Thus, the selenium atom PS derivative and PS produced by crystallising native PS (see the detailed description below) are provided as crystallised proteins suitable for X-ray diffraction analysis.

The crystals may be grown by any suitable method, e.g. the hanging drop method.

The above aspects of the invention, both singly and in combination, all contribute to features of the invention which are advantageous.

The provision of the crystal structure of PS allows a novel approach for drug discovery for modulators of this enzyme. Accordingly, the invention provides a computer-based method of rational drug design which comprises:

providing the structure of the PS as defined by the coordinates of Table 1;

providing the structure of a candidate modulator molecule;

-6-

and

fitting the structure of the candidate modulator molecule to the structure of the PS of Table 1.

5 In an alternative aspect, the method of the invention may utilise the coordinates of atoms of interest of the PS which are in the vicinity of a putative substrate and/or co-factor binding regions in order to model the pocket in which the substrate or co-factor binds. These coordinates may be used to define a space which is
10 then screened "*in silico*" against a candidate modulator molecule. Thus the invention provides a computer-based method of rational drug design which comprises:

providing the coordinates of at least two atoms of the PS of Table 1 ("selected coordinates");

15 providing the structure of a candidate modulator molecule; and

fitting the structure of the candidate modulator molecule to the selected coordinates of the PS.

20 In practice, it will be desirable to model a sufficient number of atoms of the PS as defined by the coordinates of Table 1 which represent a binding pocket. Binding pockets and other features of the interaction of PS with co-factor are described in the detailed description. Thus, in this embodiment of the invention,
25 there will preferably be provided the coordinates of at least 5, preferably at least 10, more preferably at least 50 and even more preferably at least 100 selected atoms of the PS structure.

Our structure of PS has allowed us to identify particular sites
30 of interaction of Mg^{2+} , ATP, pantoate and β -alanine. The selected coordinates preferably include at least one of the coordinates defining these particular sites. Residues providing some of these sites include Pro28, Met30, His34, Asp35, Gly36, His37, Leu40, Asn58, Gln61, Phe62, Tyr71, Arg123, His126, Ile133,

-7-

Vall134, Leu137, Lys151, Gln155, Met178, Ala185, Leu186, Ser187, Ser188, and Arg189.

As discussed in the detailed description, we believe that ATP
5 interacts with one or more of Met30, His34, Asp35, Gly36, His37, Leu40, Lys151, Met178, Ala185, Leu186, Ser187, Ser188, and Arg189; Mg^{2+} interacts with either or both of Tyr71 and Ser188; pantoate interacts with one or more of Pro28, Met30, Asn58, Gln61, Ile133, Vall134, Leu137, and Gln155; and β -alanine
10 interacts with one or more of Met30, Phe62, Tyr71, Arg123, and His126.

In another aspect, the method of the invention may utilise a sub-domain of interest of the PS which is in the vicinity of a region
15 which binds substrate or co-factor. Thus, the invention provides a computer-based method of rational drug design which comprises:
providing the coordinates of at least a sub-domain of the PS;
providing the structure of a candidate modulator molecule;
20 and
fitting the structure of the candidate modulator molecule to the coordinates of the PS sub-domain provided.

Brief Description of the Drawings

25

Fig. 1 shows schematically the pathway for the synthesis of pantothenic acid,

Figs. 2a-c show the general structure of PS, being respectively (a) a "cartoon" of the dimer, (b) a schematic
30 diagram of the monomer topology with numbering of secondary structures, and (c) a schematic plot of hydrogen bonding patterns between secondary structures,
Fig. 3 is a stereo pair of images showing schematically the core of the dimerisation interface, and

-8-

Fig. 4 shows a Connolly surface generated around the proposed PS active sites.

Detailed Description of the Invention

5

By "fitting", it is meant determining by automatic, or semi-automatic means, interactions between at least one atom of the candidate and at least one atom of the PS, and calculating the extent to which such an interaction is stable. Interactions include attraction and repulsion, brought about by charge, steric considerations and the like. Various computer-based methods for fitting are described further herein.

By "sub-domain" is meant at least one (e.g. one, two, three or four) complete element(s) of secondary structure, i.e. an alpha helix or a beta sheet, as described in the detailed description below.

Table 1 gives atomic coordinate data for PS (which we have crystallised as a dimer) and associated water molecules. In Table 1 "Atom type" refers to the respective element, the first letter defining the element; "X, Y, Z" define, with respect to the crystallographic axes, the atomic position (in Å) of the respective atom; "Occ." is the occupancy of the atom in the respective position; and "B" is a temperature factor (in Å²) which accounts for movement of the atom around its atomic centre.

Particular regions of the PS include those identified as putative substrate or cofactor binding regions based on the data provided in Table 1.

As indicated above, modulators of PS may be inhibitors of the enzyme or compounds which affect its specificity or activity in relation to pantoate in other ways. The invention is

-9-

particularly suitable for the design, screening and development of PS inhibitor components. It is thus a preferred aspect of the invention that modulators are inhibitors.

5

The step of providing the structure of a candidate modulator molecule may involve selecting the compound by computationally screening a database of compounds for interaction with the active site. For example, a 3-D descriptor for the potential modulator may be derived, the descriptor including geometric and functional constraints derived from the architecture and chemical nature of the active site. The descriptor may then be used to interrogate the compound database, a potential modulator being a compound that has a good match to the features of the descriptor. In effect, the descriptor is a type of virtual pharmacophore.

10

In any event, the determination of the three-dimensional structure of PS provides a basis for the design of new and specific ligands for PS. For example, knowing the three-dimensional structure of PS, computer modelling programs may be used to design different molecules expected to interact with possible or confirmed active sites, such as binding sites or other structural or functional features of PS.

20

25

More specifically, a potential modulator of PS activity can be examined through the use of computer modelling using a docking program such as GRAM, DOCK, or AUTODOCK (see Walters et al., *Drug Discovery Today*, Vol.3, No.4, (1998), 160-178, and Dunbrack et al., *Folding and Design*, 2, (1997), 27-42) to identify potential inhibitors of PS. This procedure can include computer fitting of potential inhibitors to PS to ascertain how well the shape and the chemical structure of the potential inhibitor will bind to the enzyme.

30

-10-

Also computer-assisted, manual examination of the active site structure of PS may be performed. The use of programs such as GRID (Goodford, *J. Med. Chem.*, 28, (1985), 849-857) - a
5 program that determines probable interaction sites between molecules with various functional groups and the enzyme surface - may also be used to analyse the active site to predict partial structures of inhibiting compounds.

10 Computer programs can be employed to estimate the attraction, repulsion, and steric hindrance of the two binding partners (e.g. the PS and a potential inhibitor). Generally the tighter the fit, the fewer the steric hindrances, and the greater the attractive forces, the more potent the potential
15 modulator, since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug, the more likely it is that the drug will not interact with other proteins as well. This will tend to minimise potential side-effects due to unwanted
20 interactions with other proteins.

In a further aspect, the present invention provides a method for identifying a candidate modulator (e.g. potential inhibitor) of PS comprising the steps of:

25 employing a three-dimensional structure of PS, or at least one sub-domain thereof, to characterise at least one PS active site, the three-dimensional structure being defined by atomic coordinate data according to Table 1; and
identifying the candidate modulator by designing or
30 selecting a compound for interaction with the active site.

If more than one PS active site is characterised and a plurality of respective compounds are designed or selected, the modulator may be formed by linking the respective compounds

-11-

into a larger compound which maintains the relative positions and orientations of the respective compounds at the active sites. The larger compound may be formed as a real molecule or by computer modelling.

5

The step of identifying the candidate modulator may involve selecting the compound by computationally screening a database of compounds for interaction with the active site.

10 In another aspect, in place of *in silico* methods, high throughput screening of compounds to select compounds with binding activity may be undertaken, and those compounds which show binding activity may be selected as possible candidate modulators, and further crystallized with PS (e.g. by co-crystallization or by soaking) for X-ray analysis. The resulting X-ray structure may be compared with that of Table 1 for a variety of purposes. For example, where the contacts made by such compounds overlap with those made by pantoate, novel molecules comprising residues which contain contacts of both pantoate and the other compound may be provided.

Having designed or selected possible binding candidate modulators by determining those which have favourable fitting properties (e.g. strong attraction between candidate and PS), these can then be screened for activity. Consequently, the method preferably further comprises the steps of:

25 obtaining or synthesising the candidate modulator; and contacting the candidate modulator with PS to determine the ability of the candidate modulator to interact with PS.

30

More preferably, in the latter step the candidate modulator is contacted with PS under conditions to determine its function.

For example, in the contacting step above the candidate

-12-

modulator is contacted with PS in the presence of a substrate, and typically a buffer, to determine the ability of said candidate modulator to inhibit PS. The substrate may be e.g. pantoic acid (or a salt thereof), β -alanine (or a salt thereof), or ATP. So, for example, an assay mixture for PS
5 may be produced which comprises the candidate modulator, substrate and buffer.

10 Instead of, or in addition to, performing such an assay, the method may comprise the further steps of:
obtaining or synthesising said candidate modulator;
forming a complex of PS and said candidate modulator; and
analysing said complex by X-ray crystallography to
15 determine the ability of said candidate modulator to interact with PS. Detailed structural information can then be obtained about the binding of the candidate modulator to PS, and in the light of this information adjustments can be made to the structure or functionality of the candidate modulator, e.g. to improve binding to the active site. The above steps may be
20 repeated and re-repeated as necessary.

In another aspect, the invention relates to a method of determining three dimensional structures of PS homologues of unknown structure by utilising the structural coordinates of
25 Table 1.

For example, if X-ray crystallographic or NMR spectroscopic data is provided for a PS homologue of unknown structure, the structure of PS as defined by Table 1 may be used to interpret
30 that data to provide a likely structure for the PS homologue by techniques which are well known in the art, e.g. phase modelling in the case of X-ray crystallography.

One embodiment of the method comprises the steps of:

-13-

(a) aligning a representation of an amino acid sequence of a PS homologue of unknown structure with the amino acid sequence of PS to match homologous regions of the amino acid sequences;

5 (b) modelling the structure of the matched homologous regions of the PS of unknown structure on the structure as defined by Table 1 of the corresponding regions of PS; and

10 (c) determining a conformation (e.g. so that favourable interactions are formed within the PS of unknown structure and/or so that a low energy conformation is formed) for the PS of unknown structure which substantially preserves the structure of said matched homologous regions.

15 The term "homologous regions" describes amino acid residues in two sequences that are identical or have similar (e.g. aliphatic, aromatic, polar, negatively charged, or positively charged) side-chain chemical groups. Identical and similar residues in homologous regions are sometimes described as being respectively "invariant" and "conserved" by those
20 skilled in the art.

Preferably one or all of steps (a) to (c) are performed by computer modelling. Homology modelling is a technique that is well known to those skilled in the art (see e.g. Greer,
25 *Science*, Vol. 228, (1985), 1055, and Blundell et al., *Eur. J. Biochem*, Vol. 172, (1988), 513).

30 In general, comparison of amino acid sequences is accomplished by aligning the amino acid sequence of a polypeptide of a known structure with the amino acid sequence of the polypeptide of unknown structure. Amino acids in the sequences are then compared and groups of amino acids that are homologous are grouped together. This method detects conserved regions of the polypeptides and accounts for amino

-14-

acid insertions or deletions.

Homology between amino acid sequences can be determined using commercially available algorithms. The programs *BLAST*, *gapped*
5 *BLAST*, *BLASTN* and *PSI-BLAST* (provided by the National Center for Biotechnology Information) are widely used in the art for this purpose, and can align homologous regions of two amino acid sequences.

- 10 Once the amino acid sequences of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in a computer representation of the polypeptide with known structure are transferred to the corresponding amino acids of the polypeptide whose structure
15 is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure.
- 20 The structures of amino acids located in non-conserved regions may be assigned manually by using standard peptide geometries or by molecular simulation techniques, such as molecular dynamics. The final step in the process is accomplished by refining the entire structure using molecular dynamics and/or
25 energy minimization.

The aspects of the invention described herein which utilise the PS structure *in silico* may be equally applied to homologue models of PS obtained by the above aspect of the invention,
30 and this application forms a further aspect of the present invention. Thus having determined a conformation of a PS by the method described above, such a conformation may be used in a computer-based method of rational drug design as described herein.

-15-

In another aspect, the invention includes a compound which is identified as a modulator (preferably an inhibitor) of PS by the methods of the invention described above.

5

Following identification of an inhibitor compound, it may be manufactured and/or used in the preparation, i.e. manufacture or formulation, of a composition such as a medicament, pharmaceutical composition or drug. These may be administered to individuals.

10

Thus, the present invention extends in various aspects not only to an inhibitor as provided by the invention, but also a pharmaceutical composition, medicament, drug or other composition comprising such an inhibitor e.g. for treatment (which may include preventative treatment) of disease such as microbial infection; a method comprising administration of such a composition to a patient, e.g. for treatment of disease such as microbial infection; use of such an inhibitor in the manufacture of a composition for administration, e.g. for treatment of disease such as microbial infection; and a method of making a pharmaceutical composition comprising admixing such an inhibitor with a pharmaceutically acceptable excipient, vehicle or carrier, and optionally other ingredients.

25

In a further aspect, the invention provides a method for determining the structure of a modulator of PS bound to PS, said method comprising:

30

providing a crystal of PS according to the invention; soaking the crystal with said modulator; and determining the structure of said PS-modulator complex.

Alternatively, the PS and modulator may be co-crystallized.

-16-

In either case, pantoate, β -alanine and/or pantothenate or an analogue thereof may optionally be present.

Having obtained and characterized a modulator compound
5 according to the invention, the invention further provides a method for modulating the activity of PS which method comprises:

providing PS under conditions where, in the absence of modulator, the PS is able to synthesize pantothenate from
10 pantoate;

providing a modulator compound; and

determining the extent to which the activity of PS is altered by the presence of said compound.

15 In another aspect, the present invention provides systems, particularly a computer system, intended to generate structures and/or perform rational drug design for PS or a complex of PS and a potential modulator, the systems containing either (a) atomic coordinate data according to
20 Table 1, said data defining the three-dimensional structure of PS or at least one sub-domain thereof, or (b) structure factor data for PS, said structure factor data being derivable from the atomic coordinate data of Table 1.

25 In a further aspect, the present invention provides computer readable media with either (a) atomic coordinate data according to Table 1 recorded thereon, said data defining the three-dimensional structure of PS, at least one atom or at
30 least one sub-domain thereof, or (b) structure factor data for PS recorded thereon, the structure factor data being derivable from the atomic coordinate data of Table 1.

As used herein, "computer readable media" refers to any medium or media which can be read and accessed directly by a

-17-

computer. Such media include, but are not limited to:
magnetic storage media such as floppy discs, hard disc storage
medium and magnetic tape; optical storage media such as
optical discs or CD-ROM; electrical storage media such as RAM
5 and ROM; and hybrids of these categories such as
magnetic/optical storage media.

By providing such computer readable media, the atomic
coordinate data can be routinely accessed to model PS or a
10 sub-domain thereof. For example, RASMOL (Sayle et al., *TIBS*,
Vol. 20, (1995), 374) is a publicly available computer
software package which allows access and analysis of atomic
coordinate data for structure determination and/or rational
drug design.

15 On the other hand, structure factor data, which are derivable
from atomic coordinate data (see e.g. Blundell et al., in
Protein Crystallography, Academic Press, New York, London and
San Francisco, (1976)), are particularly useful for
20 calculating e.g. difference Fourier electron density maps.

As used herein, "a computer system" refers to the hardware
means, software means and data storage means used to analyse
the atomic coordinate data of the present invention. The
25 minimum hardware means of the computer-based systems of the
present invention comprises a central processing unit (CPU),
input means, output means and data storage means. Desirably a
monitor is provided to visualise structure data. The data
storage means may be RAM or means for accessing computer
30 readable media of the sixth aspect of the invention. Examples
of such systems are microcomputer workstations available from
Silicon Graphics Incorporated and Sun Microsystems running
Unix based, Windows NT or IBM OS/2 operating systems.

-18-

In a further aspect, the invention provides a method of analysing a complex of PS and a potential modulator comprising the step of employing (i) X-ray crystallographic diffraction data from the complex and (ii) a three-dimensional structure of PS, or at least one sub-domain thereof, to generate a difference Fourier electron density map of the complex, the three-dimensional structure being defined by atomic coordinate data according to Table 1. The difference Fourier electron density map may then be analysed.

Therefore, such complexes can be crystallised and analysed using X-ray diffraction methods, e.g. according to the approach described by Greer et al., *J. of Medicinal Chemistry*, Vol. 37, (1994), 1035-1054, and difference Fourier electron density maps can be calculated based on X-ray diffraction patterns of soaked or co-crystallised PS and the solved structure of uncomplexed PS. These maps can then be analysed e.g. to determine whether and where a particular ligand binds to PS and/or changes the conformation of PS.

Electron density maps can be calculated using programs such as those from the CCP4 computing package (Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, *Acta Crystallographica*, D50, (1994), 760-763.). For map visualisation and model building programs such as "O" (Jones et al., *Acta Crystallography*, A47, (1991), 110-119) can be used.

PS Structural Characterization

We have found that the structure of a PS monomer consists of two major domains, joined at about residue 176 (Figs. 2a-c). Domain N (so called because it contains the N terminal) has an alpha-beta-alpha architecture; six parallel β -strands with 1'-

-19-

3-2-1-4-5 topology alternate with α -helices to form a Rossman fold with central β -sheet sandwiched between two layers of α -helices (Fig. 2b). The helices ($\alpha 1'$, 1, 2, 3 and 4) pack against the β -sheet in a right-handed way. The secondary structural elements have been numbered in Figs. 2a and b, with elements that are insertions or additions to the "standard" nucleotide-binding Rossman fold (discussed below under "Identification of Likely Active Sites") denoted by primes. Strand $\beta 5$ leads directly into the short β -hairpin and 3_{10} helix motif ($\beta 6$, $\beta 7$ and ϵ_{107}), which lies at the head of domain C (containing the C terminal) and is likely to be involved in phosphate binding (see below). The rest of the domain has a simple two-layer organisation: a helix-turn-helix layered above a flat sheet of three anti-parallel β -strands ($\alpha 8$ and 9 , $\beta 10$ -12). This sheet faces a prominent cleft in domain N, the predicted catalytic region (see below), making the whole structure resemble somewhat a pot (domain N) with its lid (domain C) on a hinge, a common arrangement in two-domain enzymes.

20

We have also found that the two monomers, A and B, of PS are related by a non-crystallographic quasi 2-fold rotational symmetry (NCS) axis. The dimerisation interface has a surface area of 1340 \AA^2 and the core of the interface is shown in Fig.

25

3. The centre of the nearly symmetrical dimerisation interface is unusual: below a 2-strand β -sheet (βD from A and B) Val109, Met166 and Phe168 form a hydrophobic pocket around weakly H-bonded polar clusters of Ser135, conserved Asn139 and three water molecules, one of which lies on the NCS axis.

30

Above the β -sheet Tyr108, Asp110 and Arg128 form a tight charged cluster, and the rest of the interface consists of salt bridges (His106 to Asp165; Arg11 to Asp169) and extensive water-mediated H-bonding interactions.

-20-

The average B-factor of monomer B is about 4 Å² greater than that of A, which on the whole contains fewer disordered stretches. Also conformational differences between the monomers which can be explained by crystal packing
5 arrangements are found at residues 173-180 and 187-193.

For residues B187-193, electron density was poor, and the apparent backbone connectivity could not be reconciled with stereochemical and Ramachandran constraints. The loop was
10 eventually modelled using the same residues from monomer A (which are well ordered), and transformed by the operation that superimposes domain C of monomer A onto monomer B. However, it is likely that residues A187-193 are only ordered because the bottom of the dimerisation region is
15 crystallographically packed tightly against this region and that the disordered seen in B is more realistic for the apo-enzyme *in vivo*.

Residues 239-244 also have entirely different but defined
20 backbone conformations in the two monomers, and this difference is not readily explained by crystal packing. However, there appears to be no functional significance in the anomaly.

25 *Solving the PS Crystal Structure*

To solve the PS crystal structure, molecular replacement was not possible because prior to our determination of the PS structure similarities between the amino acid sequence of
30 *E.coli* PS and that of proteins with known structures were not evident. Therefore, phase information needed to be obtained *ab initio*.

The phase problem was first approached by the Multiple

-21-

Isomorphous Replacement technique, and crystals of PS were soaked with a range of heavy atom salts at a range of concentrations. However, the majority of these conditions resulted in crystal damage.

5

Eventually, production of selenomethionine PS (SeMet PS) was attempted, the selenium atoms being introduced into the protein prior to crystallisation by recombinant production of the protein in the presence of L-selenomethionine. This was successfully accomplished and is discussed in more detail below. X-ray analysis was performed on PS and SeMet PS crystals.

10

1. Production and purification of PS

15

Native PS

DNA encoding the PanC gene was engineered into a pUC19 expression vector. *E.coli* cells were transformed using the plasmid.

20

Colonies of transformed cells were inoculated directly into LB medium containing ampicillin (100 mg/ml) and IPTG (70mg/ml); induction of expression was continuous. The cultures were shaken (200 rpm on an orbital shaker) overnight at 37°C, when the cells were retrieved by centrifugation of the culture medium and the cell pellet stored frozen at -80°C.

25

Selenomethionine PS

30

The same *E.coli* strain was used as for native expression, but the methionine pathway inhibition system (see van Duyne et al., *J. Mol. Biol.*, 229, (1993), 105-124) was used for selenomethionine incorporation. Cells were grown on a

-22-

minimal, defined medium (see Table 2) containing selenomethionine as well as six other amino acids, whose presence inhibits the natural pathways for methionine synthesis. A starter culture (100ml) of the same medium as above, but without selenomethionine or the inhibitory amino acids, was inoculated with transformed cells and grown at 37°C to log growth phase. 1ml of this culture was used to inoculate baffled 2/Erlemeyer flasks (250ml complete medium per flask) which were shaken at 37°C overnight and harvested as for native protein.

Purification

Harvested cells were suspended in 20-40ml TD buffer (50mM Tris/HCl pH 7.5 + 0.1mM dithiothreitol) sonicated at maximum intensity for 8 times 15 seconds, with 15 second breaks, and cell debris removed by centrifugation (30 minutes, 15000x g).

The supernatant was stirred at 4°C while $(\text{NH}_4)_2\text{SO}_4$ was added slowly over ca. 15 minutes to a final concentration of 29.1% (w/v); after a further 30 minutes of stirring, precipitated contaminants were removed by centrifugation (30 minutes, 15000x g). The solution was dialysed overnight against TD buffer (at least 2l).

The dialysed protein solution was loaded at 4°C onto an anion exchange column (Pharmacia Q-Sepharose, 16/10) and eluted with TD buffer against a NaCl gradient of 0 to 500mM in 75 minutes, at a flow rate of 5ml/min. The protein eluted between 0.21 and 0.24M NaCl. The protein-containing fractions were selected from SDS-PAGE analysis, and concentrated to ca 1ml.

The concentrated fractions were loaded at 4°C onto a size exclusion column (Pharmacia S200HR), and eluted with TD buffer

-23-

containing NaCl at 500mM. The fractions containing PS were confirmed by SDS-PAGE analysis. The fractions were pooled and dialysed overnight against TD buffer (at least 2l).

5 The dialysed protein solution was loaded at room temperature onto an affinity column (Pharmacia Blue Sepharose HiLoad 16/10) and eluted with at least five column volumes of TD buffer containing 10mM ATP. This effectively eluted all the protein, although this was not monitored directly.

10

ATP was removed from the eluant by repeated cycles (at least 5) of concentration (in a stirred cell concentrator (Amicon7 Ultrafiltration Cell) under pressure in an N₂ atmosphere) and dilution with TD buffer; ATP content was monitored by the UV spectrum (220-300nm) of the solution. The protein was finally concentrated (Ultrafree7 concentrator) to a concentration of between 20 and 30 mg/ml. At this concentration, the solution could be aliquoted and frozen directly at -80°C without damage to the protein.

20

For the purification of the SeMet protein, some precautions were taken to minimise oxidation of the selenium in the protein. The DTT concentration in all buffers was raised to 5mM, all buffers were thoroughly purged with N₂ gas before use, and the whole procedure was completed as fast as possible, within two days. The SeMet preparations of PS were subjected to Electrospray Mass Spectrometry (ESMS) to confirm the incorporation of selenomethionine during the expression.

25

30 2. Preparation of Crystals.

Crystals of PS and SeMet PS were grown using the hanging drop vapour diffusion method. Protein (20mg/ml) was mixed on a 1:1 ratio with crystallisation solution containing 4-7% (w/w)

-24-

Polyethylene Glycol 4000 and 50mM Tris/HCl buffer at pH8. Crystals formed within 2-4 days at 19°C. Crystallisation of SeMet PS, was performed using a nearly identical protocol, but additionally, 2mM DTT was added to the crystallisation solution before mixing the drop.

Crystals ideally have approximate dimensions of 600x200x50 µm. Under non-optimal conditions, crystals grow in clusters and are generally much thinner in the 3rd dimension (10-20 µm).

Crystals of PS were cryo-protected using a protocol of gradual soaking in the cryo-protectant, glycerol. A crystal was placed in 20ul of crystallisation solution, and the concentration of glycerol is gradually increased to 28% (v/v) in 4% increments.

3. Structural Determination

Multi-wavelength data sets were collected from a cryo-cooled crystal of SeMet PS, on beam line X-25 of the NSLS at Brookhaven National Laboratories on Long Island, USA. This is a high-flux station with good intensity and wavelength stability. The presence of selenomethionine in the protein was confirmed independently by electrospray mass spectrometry. Before the experiment, a large number of crystals were extensively screened for highest resolution, low mosaicity and low background scatter.

Terminal radiation-induced diffraction decay was evident in the first crystal to be exposed, which influenced data collection from the second, final SeMet crystal.

In addition to the three data sets collected from SeMet crystals, a data set was collected from a large native

-25-

crystal, which had been established to be nearly isomorphous with the SeMet crystals used. In order to have complete but also high resolution data, the same oscillation range was exposed twice, the first for measuring low resolution data (i.e. short exposures), and the second for the highest resolution possible (long exposures). All data were processed using MOSFLM (Leslie, *Joint CCP4 and EESF-EACMB Newsletter on Protein Crystallography*, Vol.26, Daresbury Laboratory, UK) and scaled with SCALA (Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, *Acta Crystallographica*, D50, (1994), 760-763).

The selenium atoms were located using the program SnB (Weeks et al., *J. of Applied Crystallography*, 32, (1999), 120-124) and their positions refined using SHARP (LaFortelle et al., *Methods in Enzymology*, 276, (1997), 472-494 and LaFortelle et al., Maximum Likelihood Refinement in a Graphical environment, with SHARP, in *CCP4 study week-end: Recent Advances in Phasing*, ed. Wilson et al., Daresbury Laboratory, UK). The final model contained 19 selenium sites which were used to provide initial phasing. Solvent flattening and phase extension techniques were used to produce an interpretable electron density map.

The program O was used for model building. The experimental, solvent flattened electron density map was readily interpretable and secondary structural elements were clearly defined in the electron density bones (calculated with MAPMAN, see Kleywegt et al., *Acta Crystallographica*, D52, (1996b), 826-828). The main chain of one monomer could be traced nearly continuously, using the secondary structure template building functionality in O, and the selenium atoms identified using SHARP providing guidance for chain-tracing.

-26-

The complete main chain model of monomer A was manually rotated to correspond with the bones of the second monomer (B). Since the relative orientation of the two domains was slightly different in monomer B, it was optimised by rigid body refinement (using REFMAC, see Murshudov et al., *Acta Crystallographica*, D53, (1997), 24-255), keeping separate the two domains (residues 1-176 and 177-283).

The model was improved by three iterated cycles of restrained and individual isotropic maximum likelihood refinement with REFMAC (40-1.7D resolution) together with manual rebuilding in O. σ_A -weighted $2F_{\text{obs}} - F_{\text{calc}}$ and $F_{\text{obs}} - F_{\text{calc}}$ maps were used (Read, *Acta Crystallographica*, A42, (1986), 140-149), the former frequently informative even when contoured at only 0.8-0.9 map standard deviations. For difficult parts of the model, maps and models resulting from simulated annealing in CNS (Brunger et al., *Acta Crystallographica*, D54, (1998), 905-921) were also considered. Ordered water molecules were modelled by automated cycles of water addition and removal by ARP (Perrakis et al., *Acta Crystallographica*, D55, (1999), 1765-1770) and refinement by REFMAC, with a final cycle of refinement with bulk solvent correction using CNS to ensure good geometry.

The final model consists of 4290 non-hydrogen protein atoms, and 384 water molecules. All residues were modelled, but electron density was poor for C-terminal residues (A283, B282-3), as well as residues B187-193; the B-factors of these residues are high, approaching 80\AA^2 . Residues A251-259, B63-68 and B251-259, though visible, are also not well ordered and have B-factors approaching 60\AA^2 . Two residues (A4 and A273) have alternative conformations, and 12 surface-exposed side chains are disordered and were modelled as the most common rotamer at zero occupancy.

-27-

Table 3 provides model parameters and refinement statistics for a version of the model which is essentially the same as that of Table 1 but contains more water molecules and also two ethanediol molecules and a Tris molecule. Residues B188-192 of this version of the model were reconstructed using BUSTER (Bricogne, *Methods in Enzymology*, 276, (1997), 361-423) in its implementation with TNT (Tronrud, *Methods in Enzymology*, 277, (1997), 306-319) instead of by the symmetry operation described above under "PS Structural Characterization". The program DDQ (van den Akker et al., *Acta Crystallographica*, D55, (1999), 206-218) was used to assess local and global accuracy and satisfactory completion of refinement, by considering difference density peaks arising from the final model. σ_A -weighted difference maps were calculated in REFMAC, excluding water molecules from the model. Quality of the model and its geometry were assessed by OOPS (Kleywegt et al., OOPS-a-daisy, *CCP4/ESF-EACBM Newsletter on Protein Crystallography*, 30, (1994), 20-24), PROCHECK (Laskowski et al., *J. Applied Crystallography*, 26, (1993), 283-291) and WHATCHECK (Hooft et al., *Nature*, 381, (1996), 272). No serious deviations from expected values are present, and warnings either correspond to well-defined justifiable features or else poorly-visible features that have high B-factors anyway. There are no Ramachandran outliers, and 92.2% of residues lie in most favoured regions of the plot.

Identification of Likely Active Sites

Having solved the PS crystal structure it is now evident that in terms of their C_α coordinates, the ATP-binding domains of (i) class I amino-acid tRNA synthetases (tRS) (i.e. EtRS from *Thermus thermophilus*, Nureki et al., *Science*, 267, (1995) 1958-1965; QtRS from *E. coli*, Perona et al., *Biochemistry*, 32,

-28-

(1993) 8758-8771; MtRS from *Thermus aquaticus*, Mechulam et al., *J. of Molecular Biology*, 294, (1999), 1287-1297; and YtRS from *Bacillus stearothermophilus*, Brick et al., *J. of Molecular Biology*, 208, (1989), 83-98), (ii)

- 5 phosphopantetheine adenylyltransferase (PPAT) from *E. coli* (Izard et al., *EMBO Journal*, 18, (1999), 2021-2030) and (iii) CTP:glycerol-3-phosphate cytidylyltransferase (CGT) from *B. subtilis* (Weber et al., *Structure with Folding and Design*, 7, (1999), 1113-1124) are structurally similar to domain N of PS.

10

More specifically, the particular class of Rossman fold which characterises tRS, CGT and PPAT consists of five β -strands in a central sheet and a cleft between β -strands β 1 and β 4 at the adenosine-binding site (see Fig. 2c). PS also has these

15 features. In addition, in all four cases strand β 5 is followed by catalytically important residues which form the KMSKS motif discussed below), and for both PS and tRS strand β 5 leads directly into the next domain.

- 20 Furthermore, two sequence motifs, HIGH and KMSKS (Barker et al., *FEBS Letters*, 145, (1982), 191-193), are conserved in tRS proteins and also in the wider superfamily. From mutational studies (First et al., in *Biochemistry*, 32, (1993), 13644-13663) these motifs are known to be involved in ATP binding:
- 25 the HIGH motif binds the adenine portion of ATP (cytidine in CGT) and the KMSKS motif stabilises the β - and γ -phosphate groups. These motifs are also found in PS and correspond respectively to residues 34-37 and 185-189.

- 30 The location of the bound ATP adenine in the structure of QtRS corresponds to within 2 to 3D of the positions of the bound nucleotides in YtRS, PPAT and CGT, i.e. in the cleft between strands β 1 and β 4 of the Rossman fold and against the top of helix α 1 (the location of the HIGH motif). When this domain

-29-

of QtRS is aligned with domain N of PS the HIGH (actually HDGH in PS) residues line up very well and the QtRS-bound ATP fits nearly perfectly into the same cleft in PS. Despite this excellent match, there is a difference in the positions of the helices ϵ_{107} (in PS) and αI (in QtRS) relative to the Rossman domain. This is the location of the KMSKS motif. However, by changing conservatively the ϕ/ψ -angles of residues Val175, Pro176, Ile177 and Met178 which form the PS inter-domain linker main chain, domain C can be rotated sufficiently to align the KMSKS residues with their QtRS counterparts and thus involve them in phosphate binding.

Fig. 4 shows a Connolly surface generated around the proposed PS active sites. The skilled person would immediately recognise that residues shown in the figure would be involved in respective interactions with Mg^{2+} , ATP, pantoate and β -alanine.

The Connolly surface opens besides the ATP ribose group and the walls are formed by fully conserved residues, which are largely hydrophobic but include some polar groups. The catalytically essential Mg^{2+} ion is shown at its most likely position where it is bound to OG_{Ser188} , OH_{Tyr71} , $O^{\beta 1}_{ATP}$ and $O^{\gamma 1}_{ATP}$. This is also the proposed Mg^{2+} binding position in PPAT.

Slightly more speculatively, the most favourable conformer of pantoate is shown positioned in a cavity where it appears to satisfy the hydrophobic and hydrogen-bonding interactions of the substrate, as well as being suitably positioned for attack on ATP.

Binding positions for β -alanine may also be proposed, but with less certainty than the binding positions of ATP and pantoate. For example, the β -alanine carboxylate may bind in a conserved, positively charged pocket to Arg123, with Met30,

-30-

Phe62 and Tyr71 providing a hydrophobic patch to accommodate the two β -alanine methylene groups, and His126 being suitably positioned to deprotonate the NH_3^+ group.

- 5 A list of the residues which line the binding pockets is provided in Table 4. Some or all of these residues may be used to model PS active sites in the various aspects of the invention discussed above.

10 *Structure-Based Drug Design*

- Determination of the 3D structure of PS provides important information about the likely active sites of PS, particularly when comparisons are made with similar enzymes. This
15 information may then be used for rational design of PS inhibitors, e.g. by computational techniques which identify possible binding ligands for the active sites, by enabling linked-fragment approaches to drug design, and by enabling the identification and location of bound ligands using X-ray
20 crystallographic analysis. These techniques are discussed in more detail below.

- Greer et al. mentioned above describes an iterative approach to ligand design based on repeated sequences of computer
25 modelling, protein-ligand complex formation and X-ray analysis. Thus novel thymidylate synthase inhibitor series were designed de novo by Greer et al., and PS inhibitors may also be designed in the this way. More specifically, using e.g. GRID on the solved 3D structure of PS, a ligand (e.g. a
30 potential inhibitor) for PS may be designed that complements the functionalities of the PS active site(s). The ligand can then be synthesised, formed into a complex with PS, and the complex then analysed by X-ray crystallography to identify the actual position of the bound ligand. The structure and/or

-31-

functional groups of the ligand can then be adjusted, if necessary, in view of the results of the X-ray analysis, and the synthesis and analysis sequence repeated until an optimised ligand is obtained. Related approaches to structure-based drug design are also discussed in Bohacek et al., *Medicinal Research Reviews*, Vol.16, (1996), 3-50.

As a result of the determination of the PS 3D structure, more purely computational techniques for rational drug design may also be used to design PS inhibitors (for an overview of these techniques see e.g. Walters et al. mentioned above). For example, automated ligand-receptor docking programs (discussed e.g. by Jones et al. in *Current Opinion in Biotechnology*, Vol.6, (1995), 652-656) which require accurate information on the atomic coordinates of target receptors may be used to design potential PS inhibitors.

Linked-fragment approaches to drug design also require accurate information on the atomic coordinates of target receptors. The basic idea behind these approaches is to determine (computationally or experimentally) the binding locations of plural ligands to a target molecule, and then construct a molecular scaffold to connect the ligands together in such a way that their relative binding positions are preserved. The ligands may be provided computationally and modelled in a computer system, or provided in an experimental setting, wherein crystals according to the invention are provided and a plurality of ligands soaked separately or in mixed pools into the crystal prior to X-ray analysis and determination of their location.

The binding site of two or more ligands are determined and may be connected to form a potential lead compound that can be further refined using e.g. the iterative technique of Greer et

-32-

al. For a virtual linked-fragment approach see Verlinde et al., *J. of Computer-Aided Molecular Design*, 6, (1992), 131-147, and for NMR and X-ray approaches see Shuker et al., *Science*, 274, (1996), 1531-1534 and Stout et al., *Structure*, 6, (1998), 839-848. The use of these approaches to design PS inhibitors is made possible by the determination of the PS structure.

Many of the techniques and approaches to structure-based drug design described above rely at some stage on X-ray analysis to identify the binding position of a ligand in a ligand-protein complex. A common way of doing this is to perform X-ray crystallography on the complex, produce a difference Fourier electron density map, and associate a particular pattern of electron density with the ligand. However, in order to produce the map (as explained e.g. by Blundell et al. mentioned above) it is necessary to know beforehand the protein 3D structure (or at least the protein structure factors). Therefore, determination of the PS structure also allows difference Fourier electron density maps of PS-ligand complexes to be produced, which can greatly assist the process of rational drug design.

The approaches to structure-based drug design described above all require initial identification of possible compounds for interaction with target bio-molecule (in this case PS). Sometimes these compounds are known e.g. from the research literature. However, when they are not, or when novel compounds are wanted, a first stage of the drug design program may involve computer-based *in silico* screening of compound databases (such as the Cambridge Structural Database) with the aim of identifying compounds which interact with the active site or sites of the target bio-molecule. Screening selection criteria may be based on pharmacokinetic properties such as

-33-

metabolic stability and toxicity. However, determination of the PS structure allows the architecture and chemical nature of each PS active site to be identified, which in turn allows the geometric and functional constraints of a descriptor for the potential modulator of PS activity to be derived. The descriptor is, therefore, a type of virtual 3-D pharmacophore, which can also be used as selection criteria or filter for database screening.

Compounds which have a chemical structure selected using the methods of the invention described herein, wherein said compounds are PS modulators, form a further aspect of the invention. Such compounds may be used in methods of medical treatments, such as in the treatment of bacterial infections in the human or animal body. The compounds may be used alone or in conjunction with other anti-bacterial compounds to enhance their effect.

While the invention has been described in conjunction with the exemplary embodiments described above, many equivalent modifications and variations will be apparent to those skilled in the art when given this disclosure. Accordingly, the exemplary embodiments of the invention set forth are considered to be illustrative and not limiting. Various changes to the described embodiments may be made without departing from the spirit and scope of the invention.

-34-

References

- Barker et al., *FEBS Letters*, 145, (1982), 191-193.
- Bohacek et al., *Medicinal Research Reviews*, Vol.16, (1996), 3-50.
- Brick et al., *J. of Molecular Biology*, 208, (1989), 83-98.
- Bricogne, *Methods in Enzymology*, 276, (1997), 361-423.
- Brunger et al., *Acta Crystallographica*, D54, (1998), 905-921.
- Blundell et al., in *Protein Crystallography*, Academic Press, New York, London and San Francisco, (1976).
- Blundell et al., *Eur. J. Biochem*, Vol. 172, (1988), 513.
- Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, *Acta Crystallographica*, D50, (1994), 760-763.
- Dunbrack et al., *Folding and Design*, 2, (1997), 27-42.
- First et al., in *Biochemistry*, 32, (1993), 13644-13663.
- Goodford, *J. Med. Chem.*, 28, (1985), 849-857.
- Greer, *Science*, Vol. 228, (1985), 1055.
- Greer et al., *J. of Medicinal Chemistry*, Vol. 37, (1994), 1035-1054.
- Hoofst et al., *Nature*, 381, (1996), 272.
- Izard et al., *EMBO Journal*, 18, (1999), 2021-2030.
- Jones et al., *Acta Crystallography*, A47, (1991), 110-119.
- Jones et al. in *Current Opinion in Biotechnology*, Vol.6, (1995), 652-656.
- Kleywegt et al., OOPS-a-daisy, *CCP4/ESF-EACBM Newsletter on Protein Crystallography*, 30, (1994), 20-24.
- Kleywegt et al., *Acta Crystallographica*, D52, (1996b), 826-828.
- LaFortelle et al., *Methods in Enzymology*, 276, (1997), 472-494.
- LaFortelle et al., Maximum Likelihood Refinement in a Graphical environment, with SHARP, in *CCP4 study week-end: Recent Advances in Phasing*, ed. Wilson et al., Daresbury

-35-

Laboratory, UK.

Leslie, *Joint CCP4 and EESF-EACMB Newsletter on Protein Crystallography*, Vol.26, Daresbury Laboratory, UK.

Laskowski et al., *J. Applied Crystallography*, 26, (1993), 283-291.

Mechulam et al., *J. of Molecular Biology*, 294, (1999), 1287-1297.

Miyatake et. al, *J. Biochem.*, 79, (1976), 673-678.

Murshudov et al., *Acta Crystallographica*, D53, (1997), 24-255.

Nureki et al., *Science*, 267, (1995) 1958-1965.

Perona et al., *Biochemistry*, 32, (1993) 8758-8771.

Perrakis et al., *Acta Crystallographica*, D55, (1999), 1765-1770.

Read, *Acta Crystallographica*, A42, (1986), 140-149.

Sayle et al., *TIBS*, Vol. 20, (1995), 374.

Shuker et al., *Science*, 274, (1996), 1531-1534.

Stout et al., *Structure*, 6, (1998), 839-848.

Tronrud, *Methods in Enzymology*, 277, (1997), 306-319.

van den Akker et al., *Acta Crystallographica*, D55, (1999), 206-218.

van Duyne et al., *J. Mol. Biol.*, 229, (1993), 105-124.

Verlinde et al., *J. of Computer-Aided Molecular Design*, 6, (1992), 131-147.

Walters et al., *Drug Discovery Today*, Vol.3, No.4, (1998), 160-178.

Weber et al., *Structure with Folding and Design*, 7, (1999), 1113-1124.

Weeks et al., *J. of Applied Crystallography*, 32, (1999), 120-124.

-36-

Table 1

REMARK Written by O version 6.2.1

REMARK Sun Dec 19 17:28:32 1999

5 CRYST1 66.031 78.075 77.126 90.00 103.71 90.00
 ORIGX1 1.000000 0.000000 0.000000 0.000000
 ORIGX2 0.000000 1.000000 0.000000 0.000000
 ORIGX3 0.000000 0.000000 1.000000 0.000000
 10 SCALE1 0.015144 0.000000 0.003694 0.000000
 SCALE2 0.000000 0.012808 0.000000 0.000000
 SCALE3 0.000000 0.000000 0.013346 0.000000

15 Monomer A

	Atom type	X	Y	Z	Occ.	B	Atomic No.
20	ATOM 1 N MET A 1	21.480	5.652	9.350	1.00	40.77	7
	ATOM 2 CA MET A 1	22.828	6.214	9.115	1.00	37.51	6
	ATOM 3 C MET A 1	23.471	6.721	10.394	1.00	37.12	6
	ATOM 4 O MET A 1	22.954	7.659	10.999	1.00	37.52	8
	ATOM 5 CB MET A 1	22.777	7.385	8.130	1.00	35.78	6
25	ATOM 6 CG MET A 1	24.222	7.748	7.741	1.00	33.60	6
	ATOM 7 SD MET A 1	24.158	8.882	6.335	1.00	30.36	16
	ATOM 8 CE MET A 1	23.874	10.429	7.197	1.00	27.91	6
	ATOM 9 N LEU A 2	24.565	6.125	10.835	1.00	33.76	7
	ATOM 10 CA LEU A 2	25.238	6.573	12.014	1.00	33.24	6
30	ATOM 11 C LEU A 2	26.150	7.745	11.696	1.00	32.31	6
	ATOM 12 O LEU A 2	26.856	7.637	10.679	1.00	31.54	8
	ATOM 13 CB LEU A 2	26.138	5.467	12.571	1.00	36.11	6
	ATOM 14 CG LEU A 2	25.578	4.098	12.886	1.00	40.23	6
	ATOM 15 CD1 LEU A 2	26.741	3.164	13.253	1.00	39.01	6
35	ATOM 16 CD2 LEU A 2	24.566	4.121	14.018	1.00	40.87	6
	ATOM 17 N ILE A 3	26.233	8.778	12.481	1.00	30.54	7
	ATOM 18 CA ILE A 3	27.148	9.869	12.303	1.00	30.81	6
	ATOM 19 C ILE A 3	28.090	9.801	13.509	1.00	31.50	6
	ATOM 20 O ILE A 3	27.616	9.918	14.642	1.00	31.89	8
40	ATOM 21 CB ILE A 3	26.523	11.280	12.249	1.00	31.52	6
	ATOM 22 CG1 ILE A 3	25.579	11.383	11.041	1.00	34.35	6
	ATOM 23 CG2 ILE A 3	27.610	12.348	12.227	1.00	33.27	6
	ATOM 24 CD1 ILE A 3	24.913	12.769	11.018	1.00	34.98	6
	ATOM 25 N ILE A 4	29.350	9.493	13.296	1.00	26.66	7
45	ATOM 26 CA ILE A 4	30.352	9.345	14.340	1.00	27.86	6
	ATOM 27 C ILE A 4	31.314	10.510	14.337	1.00	28.36	6
	ATOM 28 O ILE A 4	31.896	10.956	13.322	1.00	26.38	8
	ATOM 29 CB ILE A 4	31.105	7.998	14.143	1.00	27.57	6
	ATOM 30 CG1 ILE A 4	30.125	6.847	13.972	0.50	27.40	6
50	ATOM 31 CG2 ILE A 4	32.067	7.779	15.312	0.50	26.53	6
	ATOM 32 CD1 ILE A 4	29.201	6.526	15.113	0.50	28.00	6
	ATOM 33 N GLU A 5	31.633	11.053	15.537	1.00	25.12	7
	ATOM 34 CA GLU A 5	32.526	12.186	15.655	1.00	28.91	6
	ATOM 35 C GLU A 5	33.843	11.934	16.357	1.00	26.18	6
55	ATOM 36 O GLU A 5	34.724	12.779	16.300	1.00	27.45	8
	ATOM 37 CB GLU A 5	31.769	13.303	16.441	1.00	31.10	6
	ATOM 38 CG GLU A 5	30.611	13.871	15.627	1.00	34.62	6
	ATOM 39 CD GLU A 5	29.795	14.929	16.355	1.00	40.38	6
	ATOM 40 OE1 GLU A 5	30.263	15.579	17.306	1.00	41.78	8
60	ATOM 41 OE2 GLU A 5	28.625	15.153	15.971	1.00	43.11	8
	ATOM 42 N THR A 6	33.976	10.823	17.094	1.00	27.41	7
	ATOM 43 CA THR A 6	35.188	10.587	17.848	1.00	27.21	6
	ATOM 44 C THR A 6	35.969	9.345	17.384	1.00	26.94	6
	ATOM 45 O THR A 6	35.294	8.397	16.960	1.00	25.74	8
65	ATOM 46 CB THR A 6	34.867	10.400	19.351	1.00	29.81	6
	ATOM 47 OG1 THR A 6	34.175	9.170	19.608	1.00	30.13	8
	ATOM 48 CG2 THR A 6	33.967	11.528	19.852	1.00	29.59	6
	ATOM 49 N LEU A 7	37.249	9.359	17.679	1.00	27.76	7
	ATOM 50 CA LEU A 7	38.052	8.175	17.280	1.00	27.99	6
70	ATOM 51 C LEU A 7	37.684	6.899	18.006	1.00	29.61	6
	ATOM 52 O LEU A 7	37.546	5.845	17.381	1.00	26.94	8
	ATOM 53 CB LEU A 7	39.526	8.515	17.460	1.00	28.02	6
	ATOM 54 CG LEU A 7	40.011	9.725	16.678	1.00	31.71	6

-37-

	ATOM	55	CD1	LEU	A	7	41.523	9.840	16.799	1.00	34.04	6
	ATOM	56	CD2	LEU	A	7	39.612	9.641	15.219	1.00	32.76	6
	ATOM	57	N	PRO	A	8	37.434	6.913	19.313	1.00	30.58	7
5	ATOM	58	CA	PRO	A	8	37.081	5.687	20.013	1.00	29.86	6
	ATOM	59	C	PRO	A	8	35.814	5.062	19.505	1.00	28.23	6
	ATOM	60	O	PRO	A	8	35.701	3.845	19.394	1.00	25.90	8
	ATOM	61	CB	PRO	A	8	37.001	6.107	21.485	1.00	31.83	6
	ATOM	62	CG	PRO	A	8	37.816	7.345	21.593	1.00	31.44	6
10	ATOM	63	CD	PRO	A	8	37.601	8.053	20.243	1.00	30.62	6
	ATOM	64	N	LEU	A	9	34.754	5.838	19.239	1.00	27.49	7
	ATOM	65	CA	LEU	A	9	33.489	5.349	18.746	1.00	28.03	6
	ATOM	66	C	LEU	A	9	33.625	4.896	17.281	1.00	25.69	6
	ATOM	67	O	LEU	A	9	32.960	3.907	16.978	1.00	26.00	8
15	ATOM	68	CB	LEU	A	9	32.376	6.393	18.920	1.00	31.67	6
	ATOM	69	CG	LEU	A	9	32.089	6.741	20.400	1.00	35.64	6
	ATOM	70	CD1	LEU	A	9	31.037	7.824	20.573	1.00	35.73	6
	ATOM	71	CD2	LEU	A	9	31.636	5.493	21.154	1.00	37.26	6
	ATOM	72	N	LEU	A	10	34.532	5.512	16.526	1.00	25.45	7
20	ATOM	73	CA	LEU	A	10	34.763	5.045	15.154	1.00	23.19	6
	ATOM	74	C	LEU	A	10	35.461	3.678	15.228	1.00	23.87	6
	ATOM	75	O	LEU	A	10	35.017	2.730	14.592	1.00	23.85	8
	ATOM	76	CB	LEU	A	10	35.577	6.082	14.350	1.00	21.87	6
	ATOM	77	CG	LEU	A	10	36.012	5.560	12.953	1.00	22.51	6
25	ATOM	78	CD1	LEU	A	10	34.829	5.397	12.007	1.00	22.75	6
	ATOM	79	CD2	LEU	A	10	37.072	6.488	12.337	1.00	23.02	6
	ATOM	80	N	ARG	A	11	36.423	3.571	16.150	1.00	25.14	7
	ATOM	81	CA	ARG	A	11	37.191	2.304	16.232	1.00	28.37	6
	ATOM	82	C	ARG	A	11	36.236	1.209	16.642	1.00	29.20	6
30	ATOM	83	O	ARG	A	11	36.288	0.113	16.066	1.00	27.74	8
	ATOM	84	CB	ARG	A	11	38.399	2.556	17.142	1.00	31.48	6
	ATOM	85	CG	ARG	A	11	39.141	1.279	17.544	1.00	36.42	6
	ATOM	86	CD	ARG	A	11	40.384	1.586	18.401	1.00	40.76	6
	ATOM	87	NE	ARG	A	11	40.948	0.327	18.857	1.00	44.29	7
35	ATOM	88	CZ	ARG	A	11	40.627	-0.524	19.819	1.00	45.48	6
	ATOM	89	NH1	ARG	A	11	39.610	-0.297	20.644	1.00	47.34	7
	ATOM	90	NH2	ARG	A	11	41.306	-1.656	20.008	1.00	45.04	7
	ATOM	91	N	GLN	A	12	35.347	1.474	17.591	1.00	26.32	7
	ATOM	92	CA	GLN	A	12	34.364	0.453	17.968	1.00	28.52	6
40	ATOM	93	C	GLN	A	12	33.550	-0.050	16.798	1.00	27.48	6
	ATOM	94	O	GLN	A	12	33.340	-1.248	16.579	1.00	25.61	8
	ATOM	95	CB	GLN	A	12	33.450	1.032	19.051	1.00	30.81	6
	ATOM	96	CG	GLN	A	12	32.364	0.022	19.483	1.00	34.43	6
	ATOM	97	CD	GLN	A	12	31.513	0.662	20.570	1.00	37.80	6
45	ATOM	98	OE1	GLN	A	12	31.804	0.354	21.743	1.00	43.75	8
	ATOM	99	NE2	GLN	A	12	30.545	1.495	20.293	1.00	38.11	7
	ATOM	100	N	GLN	A	13	32.938	0.879	16.025	1.00	25.56	7
	ATOM	101	CA	GLN	A	13	32.110	0.497	14.901	1.00	24.82	6
	ATOM	102	C	GLN	A	13	32.889	-0.235	13.804	1.00	23.46	6
50	ATOM	103	O	GLN	A	13	32.360	-1.209	13.326	1.00	24.23	8
	ATOM	104	CB	GLN	A	13	31.427	1.706	14.213	1.00	28.90	6
	ATOM	105	CG	GLN	A	13	30.471	2.397	15.154	1.00	34.73	6
	ATOM	106	CD	GLN	A	13	29.201	1.611	15.405	1.00	37.69	6
	ATOM	107	OE1	GLN	A	13	28.697	0.913	14.519	1.00	40.12	8
55	ATOM	108	NE2	GLN	A	13	28.765	1.760	16.646	1.00	39.64	7
	ATOM	109	N	ILE	A	14	34.075	0.258	13.493	1.00	21.48	7
	ATOM	110	CA	ILE	A	14	34.904	-0.413	12.482	1.00	23.36	6
	ATOM	111	C	ILE	A	14	35.252	-1.833	12.978	1.00	23.78	6
	ATOM	112	O	ILE	A	14	35.100	-2.754	12.163	1.00	24.98	8
60	ATOM	113	CB	ILE	A	14	36.157	0.388	12.154	1.00	24.05	6
	ATOM	114	CG1	ILE	A	14	35.752	1.756	11.492	1.00	23.68	6
	ATOM	115	CG2	ILE	A	14	37.152	-0.372	11.258	1.00	23.44	6
	ATOM	116	CD1	ILE	A	14	34.981	1.571	10.185	1.00	22.33	6
	ATOM	117	N	ARG	A	15	35.691	-1.946	14.210	1.00	24.68	7
65	ATOM	118	CA	ARG	A	15	36.062	-3.331	14.658	1.00	24.36	6
	ATOM	119	C	ARG	A	15	34.868	-4.230	14.500	1.00	24.62	6
	ATOM	120	O	ARG	A	15	34.925	-5.358	13.991	1.00	26.61	8
	ATOM	121	CB	ARG	A	15	36.618	-3.304	16.087	1.00	24.77	6
	ATOM	122	CG	ARG	A	15	38.037	-2.760	16.169	1.00	29.78	6
70	ATOM	123	CD	ARG	A	15	38.488	-2.556	17.609	1.00	31.54	6
	ATOM	124	NE	ARG	A	15	38.632	-3.872	18.241	1.00	34.58	7
	ATOM	125	CZ	ARG	A	15	39.603	-4.741	17.996	1.00	36.36	6
	ATOM	126	NH1	ARG	A	15	40.588	-4.484	17.142	1.00	37.87	7
	ATOM	127	NH2	ARG	A	15	39.609	-5.896	18.638	1.00	37.41	7
	ATOM	128	N	ARG	A	16	33.681	-3.788	14.925	1.00	23.16	7

-38-

	ATOM	129	CA	ARG	A	16	32.495	-4.643	14.843	1.00	24.97	6
	ATOM	130	C	ARG	A	16	32.091	-5.007	13.453	1.00	26.58	6
	ATOM	131	O	ARG	A	16	31.688	-6.112	13.134	1.00	25.54	8
5	ATOM	132	CB	ARG	A	16	31.335	-3.905	15.565	1.00	26.81	6
	ATOM	133	CG	ARG	A	16	31.739	-3.858	17.037	1.00	30.82	6
	ATOM	134	CD	ARG	A	16	30.609	-3.393	17.953	1.00	35.27	6
	ATOM	135	NE	ARG	A	16	31.145	-3.440	19.331	1.00	38.72	7
	ATOM	136	CZ	ARG	A	16	30.380	-3.407	20.431	1.00	41.50	6
10	ATOM	137	NH1	ARG	A	16	29.057	-3.350	20.279	1.00	41.64	7
	ATOM	138	NH2	ARG	A	16	30.986	-3.478	21.616	1.00	40.81	7
	ATOM	139	N	LEU	A	17	32.236	-4.016	12.503	1.00	25.60	7
	ATOM	140	CA	LEU	A	17	31.869	-4.342	11.148	1.00	25.51	6
	ATOM	141	C	LEU	A	17	32.796	-5.382	10.547	1.00	25.77	6
15	ATOM	142	O	LEU	A	17	32.287	-6.296	9.882	1.00	27.72	8
	ATOM	143	CB	LEU	A	17	31.929	-3.067	10.251	1.00	26.53	6
	ATOM	144	CG	LEU	A	17	30.763	-2.131	10.574	1.00	28.03	6
	ATOM	145	CD1	LEU	A	17	31.127	-0.707	10.125	1.00	29.84	6
	ATOM	146	CD2	LEU	A	17	29.455	-2.554	9.941	1.00	30.48	6
20	ATOM	147	N	ARG	A	18	34.062	-5.187	10.811	1.00	25.72	7
	ATOM	148	CA	ARG	A	18	35.021	-6.172	10.278	1.00	26.50	6
	ATOM	149	C	ARG	A	18	34.894	-7.544	10.989	1.00	27.79	6
	ATOM	150	O	ARG	A	18	34.993	-8.564	10.329	1.00	26.32	8
	ATOM	151	CB	ARG	A	18	36.436	-5.665	10.405	1.00	28.86	6
25	ATOM	152	CG	ARG	A	18	36.506	-4.291	9.685	1.00	31.17	6
	ATOM	153	CD	ARG	A	18	37.972	-4.010	9.471	1.00	36.04	6
	ATOM	154	NE	ARG	A	18	38.502	-4.834	8.364	1.00	39.73	7
	ATOM	155	CZ	ARG	A	18	39.788	-5.197	8.409	1.00	41.34	6
	ATOM	156	NH1	ARG	A	18	40.523	-4.806	9.456	1.00	42.67	7
30	ATOM	157	NH2	ARG	A	18	40.324	-5.921	7.432	1.00	41.84	7
	ATOM	158	N	MET	A	19	34.537	-7.458	12.259	1.00	25.78	7
	ATOM	159	CA	MET	A	19	34.344	-8.735	13.010	1.00	27.53	6
	ATOM	160	C	MET	A	19	33.230	-9.524	12.371	1.00	26.64	6
	ATOM	161	O	MET	A	19	33.236	-10.747	12.181	1.00	25.81	8
35	ATOM	162	CB	MET	A	19	34.097	-8.377	14.473	1.00	24.76	6
	ATOM	163	CG	MET	A	19	33.680	-9.547	15.350	1.00	26.07	6
	ATOM	164	SD	MET	A	19	31.960	-10.075	15.286	1.00	24.59	16
	ATOM	165	CE	MET	A	19	31.123	-8.581	15.796	1.00	28.15	6
	ATOM	166	N	GLU	A	20	32.202	-8.844	11.855	1.00	28.38	7
40	ATOM	167	CA	GLU	A	20	31.083	-9.471	11.156	1.00	28.35	6
	ATOM	168	C	GLU	A	20	31.345	-9.875	9.720	1.00	31.76	6
	ATOM	169	O	GLU	A	20	30.395	-10.362	9.077	1.00	32.53	8
	ATOM	170	CB	GLU	A	20	29.874	-8.502	11.103	1.00	30.90	6
	ATOM	171	CG	GLU	A	20	29.474	-8.103	12.493	1.00	31.14	6
45	ATOM	172	N	GLY	A	21	32.531	-9.676	9.217	1.00	29.46	7
	ATOM	173	CA	GLY	A	21	32.968	-10.045	7.901	1.00	30.44	6
	ATOM	174	C	GLY	A	21	32.503	-9.016	6.844	1.00	28.10	6
	ATOM	175	O	GLY	A	21	32.465	-9.457	5.705	1.00	30.38	8
	ATOM	176	N	LYS	A	22	32.195	-7.815	7.269	1.00	27.01	7
50	ATOM	177	CA	LYS	A	22	31.684	-6.909	6.184	1.00	26.80	6
	ATOM	178	C	LYS	A	22	32.855	-6.293	5.441	1.00	26.41	6
	ATOM	179	O	LYS	A	22	33.844	-5.944	6.097	1.00	27.41	8
	ATOM	180	CB	LYS	A	22	30.773	-5.883	6.825	1.00	27.50	6
	ATOM	181	CG	LYS	A	22	29.392	-6.529	7.152	1.00	32.21	6
55	ATOM	182	CD	LYS	A	22	28.721	-5.570	8.118	1.00	37.87	6
	ATOM	183	CE	LYS	A	22	27.207	-5.752	8.159	1.00	42.38	6
	ATOM	184	NZ	LYS	A	22	26.574	-4.400	8.447	1.00	46.00	7
	ATOM	185	N	ARG	A	23	32.737	-6.159	4.128	1.00	26.60	7
	ATOM	186	CA	ARG	A	23	33.781	-5.503	3.325	1.00	27.62	6
60	ATOM	187	C	ARG	A	23	33.468	-4.008	3.350	1.00	25.54	6
	ATOM	188	O	ARG	A	23	32.293	-3.677	3.209	1.00	25.62	8
	ATOM	189	CB	ARG	A	23	33.784	-6.101	1.934	1.00	31.46	6
	ATOM	190	CG	ARG	A	23	34.506	-5.433	0.801	1.00	39.27	6
	ATOM	191	CD	ARG	A	23	34.206	-5.965	-0.610	1.00	43.15	6
65	ATOM	192	NE	ARG	A	23	35.366	-5.731	-1.466	1.00	45.63	7
	ATOM	193	CZ	ARG	A	23	36.577	-6.268	-1.262	1.00	46.18	6
	ATOM	194	NH1	ARG	A	23	36.841	-7.101	-0.272	1.00	47.31	7
	ATOM	195	NH2	ARG	A	23	37.537	-5.954	-2.117	1.00	48.28	7
	ATOM	196	N	VAL	A	24	34.412	-3.165	3.697	1.00	23.62	7
70	ATOM	197	CA	VAL	A	24	34.196	-1.743	3.900	1.00	22.06	6
	ATOM	198	C	VAL	A	24	34.785	-0.891	2.782	1.00	17.49	6
	ATOM	199	O	VAL	A	24	35.924	-1.166	2.392	1.00	18.13	8
	ATOM	200	CB	VAL	A	24	34.830	-1.279	5.218	1.00	22.91	6
	ATOM	201	CG1	VAL	A	24	34.677	0.198	5.452	1.00	24.86	6
	ATOM	202	CG2	VAL	A	24	34.173	-2.010	6.405	1.00	24.10	6

-39-

	ATOM	203	N	ALA	A	25	34.023	0.099	2.315	1.00	17.82	7
	ATOM	204	CA	ALA	A	25	34.597	0.939	1.279	1.00	18.16	6
	ATOM	205	C	ALA	A	25	34.593	2.272	2.004	1.00	18.48	6
5	ATOM	206	O	ALA	A	25	33.673	2.667	2.768	1.00	22.08	8
	ATOM	207	CB	ALA	A	25	33.863	1.032	-0.030	1.00	20.30	6
	ATOM	208	N	LEU	A	26	35.579	3.142	1.726	1.00	16.71	7
	ATOM	209	CA	LEU	A	26	35.791	4.438	2.266	1.00	16.65	6
	ATOM	210	C	LEU	A	26	35.819	5.507	1.152	1.00	17.57	6
10	ATOM	211	O	LEU	A	26	36.497	5.321	0.146	1.00	18.90	8
	ATOM	212	CB	LEU	A	26	37.120	4.628	3.038	1.00	18.22	6
	ATOM	213	CG	LEU	A	26	37.458	6.066	3.461	1.00	18.69	6
	ATOM	214	CD1	LEU	A	26	36.500	6.657	4.511	1.00	20.43	6
	ATOM	215	CD2	LEU	A	26	38.887	6.061	4.006	1.00	20.45	6
15	ATOM	216	N	VAL	A	27	35.065	6.569	1.318	1.00	16.54	7
	ATOM	217	CA	VAL	A	27	35.028	7.712	0.418	1.00	16.69	6
	ATOM	218	C	VAL	A	27	35.493	8.915	1.208	1.00	15.96	6
	ATOM	219	O	VAL	A	27	34.643	9.495	1.891	1.00	17.62	8
	ATOM	220	CB	VAL	A	27	33.636	8.038	-0.196	1.00	18.00	6
20	ATOM	221	CG1	VAL	A	27	33.738	9.238	-1.157	1.00	21.63	6
	ATOM	222	CG2	VAL	A	27	33.057	6.801	-0.869	1.00	20.05	6
	ATOM	223	N	PRO	A	28	36.728	9.403	1.100	1.00	18.63	7
	ATOM	224	CA	PRO	A	28	37.265	10.543	1.776	1.00	19.42	6
	ATOM	225	C	PRO	A	28	36.814	11.864	1.198	1.00	20.36	6
25	ATOM	226	O	PRO	A	28	36.941	11.994	-0.024	1.00	21.38	8
	ATOM	227	CB	PRO	A	28	38.775	10.466	1.589	1.00	23.04	6
	ATOM	228	CG	PRO	A	28	39.036	9.147	0.945	1.00	23.71	6
	ATOM	229	CD	PRO	A	28	37.765	8.641	0.309	1.00	19.69	6
	ATOM	230	N	THR	A	29	36.209	12.765	1.957	1.00	20.05	7
30	ATOM	231	CA	THR	A	29	35.752	14.046	1.426	1.00	20.41	6
	ATOM	232	C	THR	A	29	36.036	15.159	2.439	1.00	18.55	6
	ATOM	233	O	THR	A	29	36.271	14.922	3.618	1.00	19.34	8
	ATOM	234	CB	THR	A	29	34.254	14.069	1.053	1.00	21.16	6
	ATOM	235	OG1	THR	A	29	33.512	14.439	2.242	1.00	19.82	8
35	ATOM	236	CG2	THR	A	29	33.658	12.762	0.537	1.00	20.33	6
	ATOM	237	N	MET	A	30	35.897	16.391	2.003	1.00	20.47	7
	ATOM	238	CA	MET	A	30	35.998	17.616	2.811	1.00	20.82	6
	ATOM	239	C	MET	A	30	34.587	18.281	2.815	1.00	23.33	6
	ATOM	240	O	MET	A	30	34.465	19.488	3.115	1.00	23.42	8
40	ATOM	241	CB	MET	A	30	37.065	18.623	2.375	1.00	21.06	6
	ATOM	242	CG	MET	A	30	38.446	17.925	2.357	1.00	21.02	6
	ATOM	243	SD	MET	A	30	39.740	19.108	2.816	1.00	24.24	16
	ATOM	244	CE	MET	A	30	39.431	20.461	1.687	1.00	26.95	6
	ATOM	245	N	GLY	A	31	33.576	17.477	2.616	1.00	21.21	7
45	ATOM	246	CA	GLY	A	31	32.189	17.985	2.705	1.00	24.38	6
	ATOM	247	C	GLY	A	31	31.835	18.946	1.563	1.00	24.71	6
	ATOM	248	O	GLY	A	31	32.498	18.909	0.524	1.00	22.94	8
	ATOM	249	N	ASN	A	32	30.712	19.650	1.637	1.00	24.08	7
	ATOM	250	CA	ASN	A	32	30.269	20.550	0.552	1.00	22.88	6
50	ATOM	251	C	ASN	A	32	29.995	19.636	-0.655	1.00	22.70	6
	ATOM	252	O	ASN	A	32	30.519	19.801	-1.762	1.00	25.35	8
	ATOM	253	CB	ASN	A	32	31.269	21.654	0.253	1.00	27.38	6
	ATOM	254	CG	ASN	A	32	30.612	22.708	-0.658	1.00	31.01	6
	ATOM	255	OD1	ASN	A	32	29.390	22.842	-0.531	1.00	33.26	8
55	ATOM	256	ND2	ASN	A	32	31.392	23.283	-1.538	1.00	31.51	7
	ATOM	257	N	LEU	A	33	29.250	18.551	-0.428	1.00	22.17	7
	ATOM	258	CA	LEU	A	33	29.111	17.438	-1.343	1.00	20.92	6
	ATOM	259	C	LEU	A	33	28.300	17.796	-2.594	1.00	23.49	6
	ATOM	260	O	LEU	A	33	27.325	18.519	-2.397	1.00	25.06	8
60	ATOM	261	CB	LEU	A	33	28.479	16.200	-0.668	1.00	21.06	6
	ATOM	262	CG	LEU	A	33	29.372	15.713	0.501	1.00	21.76	6
	ATOM	263	CD1	LEU	A	33	28.821	14.431	1.108	1.00	24.92	6
	ATOM	264	CD2	LEU	A	33	30.834	15.495	0.073	1.00	21.13	6
	ATOM	265	N	HIS	A	34	28.691	17.217	-3.706	1.00	21.31	7
65	ATOM	266	CA	HIS	A	34	27.929	17.454	-4.953	1.00	19.68	6
	ATOM	267	C	HIS	A	34	27.793	16.165	-5.698	1.00	21.69	6
	ATOM	268	O	HIS	A	34	28.073	15.035	-5.218	1.00	21.01	8
	ATOM	269	CB	HIS	A	34	28.648	18.575	-5.722	1.00	20.00	6
	ATOM	270	CG	HIS	A	34	30.062	18.267	-6.078	1.00	23.69	6
70	ATOM	271	ND1	HIS	A	34	30.449	17.170	-6.770	1.00	26.07	7
	ATOM	272	CD2	HIS	A	34	31.211	18.953	-5.778	1.00	26.19	6
	ATOM	273	CE1	HIS	A	34	31.776	17.161	-6.890	1.00	27.03	6
	ATOM	274	NE2	HIS	A	34	32.262	18.221	-6.296	1.00	27.65	7
	ATOM	275	N	ASP	A	35	27.277	16.218	-6.957	1.00	20.96	7
	ATOM	276	CA	ASP	A	35	26.992	15.008	-7.685	1.00	21.21	6

-40-

	ATOM	277	C	ASP	A	35	28.213	14.132	-7.962	1.00	20.16	6
	ATOM	278	O	ASP	A	35	28.006	12.921	-8.079	1.00	22.17	8
	ATOM	279	CB	ASP	A	35	26.386	15.393	-9.061	1.00	23.09	6
5	ATOM	280	CG	ASP	A	35	24.959	15.842	-8.957	1.00	26.28	6
	ATOM	281	OD1	ASP	A	35	24.273	15.662	-7.929	1.00	27.10	8
	ATOM	282	OD2	ASP	A	35	24.439	16.326	-10.018	1.00	25.60	8
	ATOM	283	N	GLY	A	36	29.375	14.766	-8.056	1.00	21.98	7
	ATOM	284	CA	GLY	A	36	30.620	14.030	-8.244	1.00	21.77	6
10	ATOM	285	C	GLY	A	36	30.786	13.041	-7.065	1.00	22.77	6
	ATOM	286	O	GLY	A	36	31.157	11.870	-7.245	1.00	22.33	8
	ATOM	287	N	HIS	A	37	30.620	13.573	-5.849	1.00	22.48	7
	ATOM	288	CA	HIS	A	37	30.753	12.759	-4.642	1.00	19.90	6
	ATOM	289	C	HIS	A	37	29.688	11.715	-4.564	1.00	20.48	6
15	ATOM	290	O	HIS	A	37	29.886	10.568	-4.111	1.00	20.51	8
	ATOM	291	CB	HIS	A	37	30.659	13.645	-3.371	1.00	20.77	6
	ATOM	292	CG	HIS	A	37	31.604	14.773	-3.310	1.00	23.28	6
	ATOM	293	ND1	HIS	A	37	32.947	14.667	-2.929	1.00	28.53	7
	ATOM	294	CD2	HIS	A	37	31.407	16.089	-3.544	1.00	19.82	6
20	ATOM	295	CE1	HIS	A	37	33.536	15.843	-2.870	1.00	23.53	6
	ATOM	296	NE2	HIS	A	37	32.585	16.736	-3.250	1.00	26.84	7
	ATOM	297	N	MET	A	38	28.469	11.976	-5.080	1.00	19.18	7
	ATOM	298	CA	MET	A	38	27.409	10.961	-5.035	1.00	19.76	6
	ATOM	299	C	MET	A	38	27.795	9.798	-5.955	1.00	22.39	6
25	ATOM	300	O	MET	A	38	27.476	8.670	-5.614	1.00	21.94	8
	ATOM	301	CB	MET	A	38	26.038	11.520	-5.422	1.00	23.14	6
	ATOM	302	CG	MET	A	38	25.482	12.594	-4.447	1.00	25.87	6
	ATOM	303	SD	MET	A	38	25.332	11.996	-2.726	1.00	28.93	16
	ATOM	304	CE	MET	A	38	26.690	12.846	-1.980	1.00	25.74	6
30	ATOM	305	N	LYS	A	39	28.493	10.034	-7.069	1.00	19.54	7
	ATOM	306	CA	LYS	A	39	28.943	8.945	-7.921	1.00	21.23	6
	ATOM	307	C	LYS	A	39	29.995	8.090	-7.205	1.00	19.48	6
	ATOM	308	O	LYS	A	39	29.947	6.878	-7.283	1.00	19.63	8
	ATOM	309	CB	LYS	A	39	29.524	9.474	-9.236	1.00	23.04	6
35	ATOM	310	CG	LYS	A	39	29.977	8.354	-10.200	1.00	23.73	6
	ATOM	311	CD	LYS	A	39	28.831	7.464	-10.663	1.00	29.69	6
	ATOM	312	CE	LYS	A	39	29.392	6.340	-11.576	1.00	32.23	6
	ATOM	313	NZ	LYS	A	39	28.207	5.549	-12.095	1.00	35.95	7
	ATOM	314	N	LEU	A	40	30.869	8.716	-6.387	1.00	18.59	7
40	ATOM	315	CA	LEU	A	40	31.829	7.935	-5.587	1.00	19.30	6
	ATOM	316	C	LEU	A	40	31.065	7.001	-4.652	1.00	17.32	6
	ATOM	317	O	LEU	A	40	31.433	5.818	-4.467	1.00	19.58	8
	ATOM	318	CB	LEU	A	40	32.725	8.865	-4.822	1.00	20.84	6
	ATOM	319	CG	LEU	A	40	33.577	9.868	-5.641	1.00	21.98	6
45	ATOM	320	CD1	LEU	A	40	34.510	10.649	-4.714	1.00	19.78	6
	ATOM	321	CD2	LEU	A	40	34.368	9.211	-6.759	1.00	22.47	6
	ATOM	322	N	VAL	A	41	30.079	7.532	-3.957	1.00	19.06	7
	ATOM	323	CA	VAL	A	41	29.260	6.732	-3.016	1.00	18.09	6
	ATOM	324	C	VAL	A	41	28.598	5.614	-3.736	1.00	17.62	6
50	ATOM	325	O	VAL	A	41	28.537	4.470	-3.258	1.00	19.88	8
	ATOM	326	CB	VAL	A	41	28.253	7.674	-2.265	1.00	20.51	6
	ATOM	327	CG1	VAL	A	41	27.211	6.841	-1.514	1.00	21.02	6
	ATOM	328	CG2	VAL	A	41	29.010	8.629	-1.336	1.00	19.99	6
	ATOM	329	N	ASP	A	42	28.010	5.882	-4.952	1.00	18.32	7
55	ATOM	330	CA	ASP	A	42	27.355	4.768	-5.614	1.00	20.18	6
	ATOM	331	C	ASP	A	42	28.312	3.653	-5.995	1.00	20.77	6
	ATOM	332	O	ASP	A	42	27.977	2.483	-5.943	1.00	22.32	8
	ATOM	333	CB	ASP	A	42	26.667	5.238	-6.920	1.00	22.54	6
	ATOM	334	CG	ASP	A	42	25.531	6.164	-6.652	1.00	24.06	6
60	ATOM	335	OD1	ASP	A	42	24.908	6.188	-5.570	1.00	27.49	8
	ATOM	336	OD2	ASP	A	42	25.140	6.976	-7.558	1.00	30.83	8
	ATOM	337	N	GLU	A	43	29.539	4.041	-6.419	1.00	20.92	7
	ATOM	338	CA	GLU	A	43	30.528	3.015	-6.753	1.00	22.39	6
	ATOM	339	C	GLU	A	43	30.924	2.224	-5.512	1.00	21.74	6
65	ATOM	340	O	GLU	A	43	31.185	1.036	-5.623	1.00	23.66	8
	ATOM	341	CB	GLU	A	43	31.816	3.583	-7.342	1.00	23.36	6
	ATOM	342	CG	GLU	A	43	31.560	4.030	-8.792	1.00	32.68	6
	ATOM	343	CD	GLU	A	43	31.450	2.806	-9.705	1.00	34.94	6
	ATOM	344	OE1	GLU	A	43	32.113	1.776	-9.517	1.00	39.24	8
70	ATOM	345	OE2	GLU	A	43	30.590	2.908	-10.606	1.00	42.50	8
	ATOM	346	N	ALA	A	44	31.103	2.914	-4.372	1.00	21.59	7
	ATOM	347	CA	ALA	A	44	31.413	2.228	-3.131	1.00	20.24	6
	ATOM	348	C	ALA	A	44	30.241	1.299	-2.736	1.00	22.05	6
	ATOM	349	O	ALA	A	44	30.575	0.162	-2.324	1.00	23.77	8
	ATOM	350	CB	ALA	A	44	31.698	3.226	-2.025	1.00	19.63	6

-41-

	ATOM	351	N	LYS	A	45	29.033	1.800	-2.843	1.00	24.11	7
	ATOM	352	CA	LYS	A	45	27.888	0.912	-2.499	1.00	26.00	6
	ATOM	353	C	LYS	A	45	27.912	-0.215	-3.471	1.00	27.19	6
5	ATOM	354	O	LYS	A	45	27.573	-1.297	-2.970	1.00	28.01	8
	ATOM	355	CB	LYS	A	45	26.550	1.612	-2.555	1.00	28.17	6
	ATOM	356	CG	LYS	A	45	26.331	2.723	-1.544	1.00	33.53	6
	ATOM	357	CD	LYS	A	45	25.613	2.271	-0.277	1.00	40.20	6
	ATOM	358	CE	LYS	A	45	24.365	1.437	-0.586	1.00	42.16	6
10	ATOM	359	NZ	LYS	A	45	23.332	1.467	0.475	1.00	47.05	7
	ATOM	360	N	ALA	A	46	28.221	-0.250	-4.714	1.00	25.90	7
	ATOM	361	CA	ALA	A	46	28.227	-1.457	-5.529	1.00	26.79	6
	ATOM	362	C	ALA	A	46	29.360	-2.424	-5.183	1.00	29.75	6
	ATOM	363	O	ALA	A	46	29.233	-3.661	-5.395	1.00	28.75	8
15	ATOM	364	CB	ALA	A	46	28.360	-1.038	-6.984	1.00	28.50	6
	ATOM	365	N	ARG	A	47	30.492	-1.922	-4.680	1.00	26.27	7
	ATOM	366	CA	ARG	A	47	31.649	-2.782	-4.511	1.00	25.06	6
	ATOM	367	C	ARG	A	47	31.816	-3.283	-3.103	1.00	25.85	6
	ATOM	368	O	ARG	A	47	32.669	-4.158	-2.954	1.00	29.00	8
20	ATOM	369	CB	ARG	A	47	32.921	-1.993	-4.921	1.00	26.64	6
	ATOM	370	CG	ARG	A	47	32.973	-1.664	-6.407	1.00	30.45	6
	ATOM	371	CD	ARG	A	47	34.079	-0.626	-6.688	1.00	30.96	6
	ATOM	372	NE	ARG	A	47	33.831	-0.063	-8.068	1.00	36.09	7
	ATOM	373	CZ	ARG	A	47	34.612	-0.526	-9.051	1.00	37.23	6
25	ATOM	374	NH1	ARG	A	47	35.552	-1.422	-8.779	1.00	37.53	7
	ATOM	375	NH2	ARG	A	47	34.458	-0.076	-10.277	1.00	38.83	7
	ATOM	376	N	ALA	A	48	31.118	-2.729	-2.117	1.00	23.59	7
	ATOM	377	CA	ALA	A	48	31.382	-3.211	-0.762	1.00	23.32	6
	ATOM	378	C	ALA	A	48	30.099	-3.421	0.008	1.00	23.85	6
30	ATOM	379	O	ALA	A	48	29.048	-2.891	-0.355	1.00	26.50	8
	ATOM	380	CB	ALA	A	48	32.316	-2.196	-0.069	1.00	24.37	6
	ATOM	381	N	ASP	A	49	30.163	-4.115	1.146	1.00	22.20	7
	ATOM	382	CA	ASP	A	49	28.925	-4.271	1.916	1.00	26.00	6
	ATOM	383	C	ASP	A	49	28.562	-3.133	2.803	1.00	26.80	6
35	ATOM	384	O	ASP	A	49	27.400	-2.841	3.120	1.00	28.51	8
	ATOM	385	CB	ASP	A	49	29.066	-5.563	2.775	1.00	31.27	6
	ATOM	386	CG	ASP	A	49	29.809	-6.700	2.149	1.00	35.17	6
	ATOM	387	OD1	ASP	A	49	30.741	-7.285	2.759	1.00	35.30	8
	ATOM	388	OD2	ASP	A	49	29.459	-7.142	1.032	1.00	39.32	8
40	ATOM	389	N	VAL	A	50	29.551	-2.305	3.185	1.00	21.71	7
	ATOM	390	CA	VAL	A	50	29.379	-1.186	4.072	1.00	24.23	6
	ATOM	391	C	VAL	A	50	30.120	0.032	3.514	1.00	22.66	6
	ATOM	392	O	VAL	A	50	31.259	-0.150	3.088	1.00	23.46	8
	ATOM	393	CB	VAL	A	50	29.980	-1.492	5.460	1.00	28.04	6
45	ATOM	394	CG1	VAL	A	50	29.862	-0.274	6.353	1.00	30.12	6
	ATOM	395	CG2	VAL	A	50	29.310	-2.723	6.087	1.00	31.57	6
	ATOM	396	N	VAL	A	51	29.462	1.181	3.484	1.00	20.55	7
	ATOM	397	CA	VAL	A	51	30.124	2.367	2.940	1.00	18.63	6
	ATOM	398	C	VAL	A	51	30.317	3.377	4.038	1.00	19.83	6
50	ATOM	399	O	VAL	A	51	29.382	3.743	4.754	1.00	19.84	8
	ATOM	400	CB	VAL	A	51	29.292	3.029	1.830	1.00	21.12	6
	ATOM	401	CG1	VAL	A	51	29.993	4.288	1.310	1.00	22.56	6
	ATOM	402	CG2	VAL	A	51	29.015	2.098	0.666	1.00	23.68	6
	ATOM	403	N	VAL	A	52	31.527	3.878	4.198	1.00	18.34	7
55	ATOM	404	CA	VAL	A	52	31.884	4.890	5.151	1.00	18.76	6
	ATOM	405	C	VAL	A	52	32.298	6.183	4.450	1.00	20.80	6
	ATOM	406	O	VAL	A	52	33.147	6.104	3.559	1.00	21.14	8
	ATOM	407	CB	VAL	A	52	33.088	4.473	6.034	1.00	20.37	6
	ATOM	408	CG1	VAL	A	52	33.539	5.585	6.978	1.00	19.87	6
60	ATOM	409	CG2	VAL	A	52	32.719	3.217	6.820	1.00	21.14	6
	ATOM	410	N	VAL	A	53	31.712	7.325	4.777	1.00	18.75	7
	ATOM	411	CA	VAL	A	53	32.134	8.568	4.131	1.00	18.32	6
	ATOM	412	C	VAL	A	53	32.759	9.411	5.215	1.00	18.55	6
	ATOM	413	O	VAL	A	53	32.055	9.630	6.225	1.00	19.86	8
65	ATOM	414	CB	VAL	A	53	30.949	9.327	3.473	1.00	18.40	6
	ATOM	415	CG1	VAL	A	53	31.462	10.680	2.967	1.00	20.65	6
	ATOM	416	CG2	VAL	A	53	30.322	8.469	2.396	1.00	17.69	6
	ATOM	417	N	SER	A	54	33.913	9.963	4.996	1.00	16.45	7
	ATOM	418	CA	SER	A	54	34.482	10.911	5.946	1.00	20.30	6
70	ATOM	419	C	SER	A	54	34.280	12.349	5.478	1.00	21.22	6
	ATOM	420	O	SER	A	54	34.281	12.545	4.254	1.00	18.83	8
	ATOM	421	CB	SER	A	54	35.971	10.631	6.156	1.00	21.31	6
	ATOM	422	OG	SER	A	54	36.695	10.788	4.949	1.00	21.56	8
	ATOM	423	N	ILE	A	55	33.909	13.223	6.394	1.00	21.28	7
	ATOM	424	CA	ILE	A	55	33.699	14.621	6.108	1.00	19.86	6

-42-

	ATOM	425	C	ILE	A	55	34.649	15.356	7.100	1.00	20.76	6
	ATOM	426	O	ILE	A	55	34.344	15.342	8.300	1.00	22.84	8
	ATOM	427	CB	ILE	A	55	32.273	15.102	6.291	1.00	21.61	6
5	ATOM	428	CG1	ILE	A	55	31.333	14.422	5.255	1.00	21.20	6
	ATOM	429	CG2	ILE	A	55	32.222	16.614	6.139	1.00	22.98	6
	ATOM	430	CD1	ILE	A	55	29.854	14.691	5.584	1.00	24.15	6
	ATOM	431	N	PHE	A	56	35.723	15.883	6.577	1.00	17.70	7
	ATOM	432	CA	PHE	A	56	36.699	16.589	7.404	1.00	18.93	6
10	ATOM	433	C	PHE	A	56	37.459	17.589	6.579	1.00	20.83	6
	ATOM	434	O	PHE	A	56	38.263	17.314	5.680	1.00	21.50	8
	ATOM	435	CB	PHE	A	56	37.671	15.557	8.060	1.00	17.73	6
	ATOM	436	CG	PHE	A	56	38.721	16.209	8.950	1.00	19.66	6
	ATOM	437	CD1	PHE	A	56	38.297	16.881	10.098	1.00	20.08	6
	ATOM	438	CD2	PHE	A	56	40.059	16.144	8.616	1.00	20.24	6
15	ATOM	439	CE1	PHE	A	56	39.261	17.479	10.909	1.00	19.99	6
	ATOM	440	CE2	PHE	A	56	41.029	16.743	9.433	1.00	20.35	6
	ATOM	441	CZ	PHE	A	56	40.591	17.409	10.573	1.00	21.50	6
	ATOM	442	N	VAL	A	57	37.284	18.883	6.949	1.00	21.60	7
20	ATOM	443	CA	VAL	A	57	38.009	19.978	6.334	1.00	23.17	6
	ATOM	444	C	VAL	A	57	39.362	20.006	7.039	1.00	25.23	6
	ATOM	445	O	VAL	A	57	39.473	20.469	8.172	1.00	24.88	8
	ATOM	446	CB	VAL	A	57	37.247	21.325	6.458	1.00	23.78	6
	ATOM	447	CG1	VAL	A	57	38.051	22.403	5.763	1.00	24.08	6
25	ATOM	448	CG2	VAL	A	57	35.853	21.178	5.874	1.00	23.56	6
	ATOM	449	N	ASN	A	58	40.343	19.429	6.377	1.00	24.28	7
	ATOM	450	CA	ASN	A	58	41.667	19.181	6.907	1.00	22.31	6
	ATOM	451	C	ASN	A	58	42.545	20.385	6.858	1.00	23.05	6
	ATOM	452	O	ASN	A	58	43.072	20.747	5.806	1.00	24.44	8
30	ATOM	453	CB	ASN	A	58	42.250	18.045	6.040	1.00	21.07	6
	ATOM	454	CG	ASN	A	58	43.684	17.738	6.385	1.00	22.18	6
	ATOM	455	OD1	ASN	A	58	44.133	17.942	7.521	1.00	23.39	8
	ATOM	456	ND2	ASN	A	58	44.431	17.254	5.415	1.00	20.86	7
	ATOM	457	N	PRO	A	59	42.863	21.002	8.000	1.00	24.30	7
35	ATOM	458	CA	PRO	A	59	43.727	22.187	7.996	1.00	25.81	6
	ATOM	459	C	PRO	A	59	45.060	22.042	7.348	1.00	26.27	6
	ATOM	460	O	PRO	A	59	45.679	22.957	6.784	1.00	27.28	8
	ATOM	461	CB	PRO	A	59	43.869	22.509	9.493	1.00	24.50	6
	ATOM	462	CG	PRO	A	59	42.719	21.834	10.171	1.00	26.42	6
40	ATOM	463	CD	PRO	A	59	42.427	20.600	9.337	1.00	24.44	6
	ATOM	464	N	MET	A	60	45.602	20.784	7.391	1.00	27.24	7
	ATOM	465	CA	MET	A	60	46.952	20.529	6.856	1.00	28.64	6
	ATOM	466	C	MET	A	60	47.008	20.656	5.361	1.00	31.51	6
	ATOM	467	O	MET	A	60	48.101	20.868	4.822	1.00	31.68	8
45	ATOM	468	CB	MET	A	60	47.374	19.171	7.462	1.00	28.13	6
	ATOM	469	CG	MET	A	60	48.810	18.867	7.264	1.00	32.00	6
	ATOM	470	SD	MET	A	60	49.373	17.277	7.999	1.00	31.44	16
	ATOM	471	CE	MET	A	60	50.665	17.068	6.848	1.00	31.98	6
	ATOM	472	N	GLN	A	61	45.847	20.601	4.648	1.00	30.53	7
50	ATOM	473	CA	GLN	A	61	45.972	20.800	3.202	1.00	33.22	6
	ATOM	474	C	GLN	A	61	45.492	22.174	2.780	1.00	35.82	6
	ATOM	475	O	GLN	A	61	45.183	22.463	1.611	1.00	39.20	8
	ATOM	476	CB	GLN	A	61	45.264	19.567	2.566	1.00	31.83	6
	ATOM	477	CG	GLN	A	61	43.747	19.745	2.433	1.00	29.02	6
55	ATOM	478	CD	GLN	A	61	43.189	18.320	2.094	1.00	28.13	6
	ATOM	479	OE1	GLN	A	61	43.302	17.290	2.731	1.00	24.18	8
	ATOM	480	NE2	GLN	A	61	42.486	18.326	0.963	1.00	28.14	7
	ATOM	481	N	PHE	A	62	45.576	23.209	3.658	1.00	33.24	7
	ATOM	482	CA	PHE	A	62	45.219	24.574	3.275	1.00	33.76	6
60	ATOM	483	C	PHE	A	62	46.434	25.502	3.390	1.00	35.21	6
	ATOM	484	O	PHE	A	62	47.120	25.382	4.405	1.00	33.54	8
	ATOM	485	CB	PHE	A	62	44.138	25.218	4.136	1.00	31.27	6
	ATOM	486	CG	PHE	A	62	42.754	24.742	3.809	1.00	30.27	6
	ATOM	487	CD1	PHE	A	62	42.301	23.528	4.291	1.00	29.03	6
65	ATOM	488	CD2	PHE	A	62	41.930	25.486	2.975	1.00	29.79	6
	ATOM	489	CE1	PHE	A	62	41.037	23.065	3.956	1.00	28.62	6
	ATOM	490	CE2	PHE	A	62	40.682	25.043	2.637	1.00	28.83	6
	ATOM	491	CZ	PHE	A	62	40.223	23.823	3.112	1.00	28.44	6
	ATOM	492	N	ASP	A	63	46.598	26.394	2.439	1.00	40.06	7
70	ATOM	493	CA	ASP	A	63	47.689	27.339	2.350	1.00	42.93	6
	ATOM	494	C	ASP	A	63	47.787	28.342	3.485	1.00	44.06	6
	ATOM	495	O	ASP	A	63	48.906	28.726	3.827	1.00	43.96	8
	ATOM	496	CB	ASP	A	63	47.575	28.206	1.085	1.00	47.09	6
	ATOM	497	CG	ASP	A	63	47.423	27.434	-0.198	1.00	51.39	6
	ATOM	498	OD1	ASP	A	63	47.397	26.169	-0.162	1.00	54.46	8

-43-

	ATOM	499	OD2	ASP	A	63	47.317	28.098	-1.257	1.00	52.58	8
	ATOM	500	N	ARG	A	64	46.669	28.845	3.990	1.00	43.31	7
	ATOM	501	CA	ARG	A	64	46.717	29.795	5.095	1.00	44.44	6
5	ATOM	502	C	ARG	A	64	45.451	29.635	5.923	1.00	41.86	6
	ATOM	503	O	ARG	A	64	44.424	29.201	5.428	1.00	38.21	8
	ATOM	504	CB	ARG	A	64	46.808	31.240	4.660	1.00	47.55	6
	ATOM	505	CG	ARG	A	64	48.161	31.803	4.295	1.00	52.46	6
	ATOM	506	CD	ARG	A	64	47.938	33.125	3.520	1.00	55.58	6
10	ATOM	507	NE	ARG	A	64	47.067	32.875	2.441	1.00	58.62	7
	ATOM	508	CZ	ARG	A	64	46.215	32.846	1.486	1.00	60.36	6
	ATOM	509	NH1	ARG	A	64	45.436	33.900	1.230	1.00	62.10	7
	ATOM	510	NH2	ARG	A	64	46.118	31.748	0.742	1.00	60.56	7
	ATOM	511	N	PRO	A	65	45.506	30.080	7.169	1.00	41.07	7
15	ATOM	512	CA	PRO	A	65	44.375	30.002	8.068	1.00	41.23	6
	ATOM	513	C	PRO	A	65	43.127	30.709	7.584	1.00	41.03	6
	ATOM	514	O	PRO	A	65	42.000	30.258	7.847	1.00	39.31	8
	ATOM	515	CB	PRO	A	65	44.911	30.622	9.356	1.00	42.70	6
	ATOM	516	CG	PRO	A	65	46.398	30.368	9.281	1.00	43.00	6
20	ATOM	517	CD	PRO	A	65	46.709	30.642	7.823	1.00	42.34	6
	ATOM	518	N	GLU	A	66	43.274	31.789	6.810	1.00	41.59	7
	ATOM	519	CA	GLU	A	66	42.070	32.514	6.362	1.00	42.96	6
	ATOM	520	C	GLU	A	66	41.347	31.757	5.259	1.00	40.61	6
	ATOM	521	O	GLU	A	66	40.120	31.853	5.153	1.00	38.18	8
25	ATOM	522	CB	GLU	A	66	42.463	33.934	5.932	1.00	48.02	6
	ATOM	523	CG	GLU	A	66	43.670	33.931	5.016	1.00	54.67	6
	ATOM	524	CD	GLU	A	66	44.083	35.290	4.503	1.00	59.02	6
	ATOM	525	OE1	GLU	A	66	44.156	36.244	5.323	1.00	62.04	8
	ATOM	526	OE2	GLU	A	66	44.334	35.389	3.276	1.00	60.81	8
30	ATOM	527	N	ASP	A	67	42.108	30.969	4.481	1.00	38.50	7
	ATOM	528	CA	ASP	A	67	41.447	30.178	3.439	1.00	37.14	6
	ATOM	529	C	ASP	A	67	40.655	29.082	4.122	1.00	34.07	6
	ATOM	530	O	ASP	A	67	39.529	28.761	3.792	1.00	30.58	8
	ATOM	531	CB	ASP	A	67	42.413	29.550	2.449	1.00	41.16	6
35	ATOM	532	CG	ASP	A	67	43.388	30.540	1.846	1.00	44.61	6
	ATOM	533	OD1	ASP	A	67	43.068	31.742	1.741	1.00	46.57	8
	ATOM	534	OD2	ASP	A	67	44.487	30.073	1.482	1.00	47.46	8
	ATOM	535	N	LEU	A	68	41.286	28.452	5.142	1.00	31.94	7
	ATOM	536	CA	LEU	A	68	40.581	27.433	5.887	1.00	30.62	6
40	ATOM	537	C	LEU	A	68	39.303	27.981	6.477	1.00	30.54	6
	ATOM	538	O	LEU	A	68	38.243	27.345	6.533	1.00	30.35	8
	ATOM	539	CB	LEU	A	68	41.523	26.893	7.001	1.00	29.74	6
	ATOM	540	CG	LEU	A	68	40.908	25.958	8.016	1.00	30.11	6
45	ATOM	541	CD1	LEU	A	68	40.510	24.577	7.474	1.00	30.95	6
	ATOM	542	CD2	LEU	A	68	41.899	25.712	9.149	1.00	31.60	6
	ATOM	543	N	ALA	A	69	39.345	29.225	7.012	1.00	29.90	7
	ATOM	544	CA	ALA	A	69	38.146	29.740	7.662	1.00	32.87	6
	ATOM	545	C	ALA	A	69	37.021	29.993	6.663	1.00	34.82	6
	ATOM	546	O	ALA	A	69	35.855	29.854	7.018	1.00	35.59	8
50	ATOM	547	CB	ALA	A	69	38.487	31.030	8.425	1.00	32.66	6
	ATOM	548	N	ARG	A	70	37.345	30.321	5.431	1.00	34.63	7
	ATOM	549	CA	ARG	A	70	36.337	30.625	4.423	1.00	37.34	6
	ATOM	550	C	ARG	A	70	35.777	29.350	3.803	1.00	36.74	6
	ATOM	551	O	ARG	A	70	34.726	29.502	3.165	1.00	35.73	8
55	ATOM	552	CB	ARG	A	70	36.923	31.526	3.334	1.00	38.93	6
	ATOM	553	CG	ARG	A	70	37.284	32.923	3.813	1.00	41.54	6
	ATOM	554	CD	ARG	A	70	37.555	33.855	2.643	1.00	43.19	6
	ATOM	555	NE	ARG	A	70	38.731	33.447	1.880	1.00	47.13	7
	ATOM	556	CZ	ARG	A	70	39.977	33.789	2.190	1.00	47.82	6
60	ATOM	557	NH1	ARG	A	70	40.213	34.544	3.252	1.00	51.37	7
	ATOM	558	NH2	ARG	A	70	40.984	33.371	1.435	1.00	48.98	7
	ATOM	559	N	TYR	A	71	36.419	28.197	3.875	1.00	32.87	7
	ATOM	560	CA	TYR	A	71	35.941	26.999	3.187	1.00	31.99	6
	ATOM	561	C	TYR	A	71	34.522	26.700	3.578	1.00	30.54	6
65	ATOM	562	O	TYR	A	71	34.125	26.714	4.739	1.00	30.28	8
	ATOM	563	CB	TYR	A	71	36.927	25.840	3.502	1.00	29.15	6
	ATOM	564	CG	TYR	A	71	36.753	24.730	2.482	1.00	29.96	6
	ATOM	565	CD1	TYR	A	71	37.363	24.753	1.233	1.00	30.99	6
	ATOM	566	CD2	TYR	A	71	35.931	23.658	2.815	1.00	29.82	6
70	ATOM	567	CE1	TYR	A	71	37.166	23.667	0.356	1.00	33.09	6
	ATOM	568	CE2	TYR	A	71	35.713	22.625	1.927	1.00	31.04	6
	ATOM	569	CZ	TYR	A	71	36.332	22.650	0.702	1.00	31.47	6
	ATOM	570	OH	TYR	A	71	36.163	21.647	-0.214	1.00	34.74	8
	ATOM	571	N	PRO	A	72	33.687	26.356	2.591	1.00	33.76	7
	ATOM	572	CA	PRO	A	72	32.271	26.095	2.809	1.00	35.62	6

-44-

	ATOM	573	C	PRO	A	72	31.987	24.932	3.712	1.00	36.23	6
	ATOM	574	O	PRO	A	72	32.552	23.855	3.521	1.00	37.45	8
	ATOM	575	CB	PRO	A	72	31.695	25.904	1.408	1.00	36.05	6
5	ATOM	576	CG	PRO	A	72	32.853	25.628	0.524	1.00	36.68	6
	ATOM	577	CD	PRO	A	72	34.044	26.284	1.155	1.00	35.26	6
	ATOM	578	N	ARG	A	73	31.114	25.089	4.705	1.00	35.24	7
	ATOM	579	CA	ARG	A	73	30.752	23.978	5.580	1.00	35.44	6
	ATOM	580	C	ARG	A	73	29.254	23.808	5.446	1.00	36.32	6
10	ATOM	581	O	ARG	A	73	28.544	24.827	5.569	1.00	36.64	8
	ATOM	582	CB	ARG	A	73	31.232	24.214	7.012	1.00	37.96	6
	ATOM	583	CG	ARG	A	73	32.778	24.055	6.985	1.00	38.27	6
	ATOM	584	CD	ARG	A	73	33.433	24.599	8.180	1.00	39.86	6
	ATOM	585	NE	ARG	A	73	34.854	24.417	8.347	1.00	37.69	7
15	ATOM	586	CZ	ARG	A	73	35.799	25.216	7.876	1.00	38.63	6
	ATOM	587	NH1	ARG	A	73	37.047	24.918	8.212	1.00	36.16	7
	ATOM	588	NH2	ARG	A	73	35.534	26.279	7.132	1.00	38.20	7
	ATOM	589	N	THR	A	74	28.763	22.645	5.057	1.00	34.43	7
	ATOM	590	CA	THR	A	74	27.358	22.363	4.859	1.00	34.04	6
20	ATOM	591	C	THR	A	74	27.033	20.953	5.354	1.00	32.80	6
	ATOM	592	O	THR	A	74	26.421	20.107	4.689	1.00	31.08	8
	ATOM	593	CB	THR	A	74	26.856	22.409	3.403	1.00	36.39	6
	ATOM	594	OG1	THR	A	74	27.567	21.394	2.652	1.00	38.24	8
	ATOM	595	CG2	THR	A	74	27.020	23.800	2.776	1.00	37.30	6
25	ATOM	596	N	LEU	A	75	27.405	20.714	6.616	1.00	31.90	7
	ATOM	597	CA	LEU	A	75	27.234	19.377	7.168	1.00	30.80	6
	ATOM	598	C	LEU	A	75	25.818	18.900	7.129	1.00	30.32	6
	ATOM	599	O	LEU	A	75	25.595	17.716	6.815	1.00	29.31	8
	ATOM	600	CB	LEU	A	75	27.865	19.401	8.605	1.00	32.17	6
30	ATOM	601	CG	LEU	A	75	27.986	18.001	9.219	1.00	33.15	6
	ATOM	602	CD1	LEU	A	75	28.985	17.154	8.420	1.00	33.59	6
	ATOM	603	CD2	LEU	A	75	28.401	18.093	10.663	1.00	32.87	6
	ATOM	604	N	GLN	A	76	24.793	19.692	7.502	1.00	29.90	7
	ATOM	605	CA	GLN	A	76	23.429	19.175	7.436	1.00	31.72	6
35	ATOM	606	C	GLN	A	76	23.040	18.695	6.054	1.00	28.82	6
	ATOM	607	O	GLN	A	76	22.449	17.626	5.924	1.00	30.69	8
	ATOM	608	CB	GLN	A	76	22.423	20.270	7.881	1.00	34.78	6
	ATOM	609	CG	GLN	A	76	21.016	19.720	8.042	1.00	40.38	6
	ATOM	610	CD	GLN	A	76	20.095	20.836	8.524	1.00	45.28	6
40	ATOM	611	OE1	GLN	A	76	19.111	21.196	7.859	1.00	48.24	8
	ATOM	612	NE2	GLN	A	76	20.453	21.402	9.677	1.00	47.35	7
	ATOM	613	N	GLU	A	77	23.274	19.493	5.023	1.00	26.49	7
	ATOM	614	CA	GLU	A	77	22.946	19.111	3.656	1.00	27.35	6
	ATOM	615	C	GLU	A	77	23.777	17.906	3.193	1.00	27.59	6
45	ATOM	616	O	GLU	A	77	23.263	17.064	2.463	1.00	27.03	8
	ATOM	617	CB	GLU	A	77	23.227	20.280	2.718	1.00	28.83	6
	ATOM	618	CG	GLU	A	77	22.722	19.997	1.302	1.00	32.09	6
	ATOM	619	N	ASP	A	78	25.048	17.886	3.617	1.00	26.66	7
	ATOM	620	CA	ASP	A	78	25.875	16.706	3.239	1.00	26.91	6
50	ATOM	621	C	ASP	A	78	25.226	15.431	3.735	1.00	26.68	6
	ATOM	622	O	ASP	A	78	25.042	14.448	3.018	1.00	24.38	8
	ATOM	623	CB	ASP	A	78	27.275	16.820	3.796	1.00	25.18	6
	ATOM	624	CG	ASP	A	78	28.116	17.931	3.332	1.00	28.50	6
	ATOM	625	OD1	ASP	A	78	27.681	18.573	2.312	1.00	28.92	8
55	ATOM	626	OD2	ASP	A	78	29.179	18.397	3.774	1.00	29.90	8
	ATOM	627	N	CYS	A	79	24.883	15.488	5.051	1.00	27.85	7
	ATOM	628	CA	CYS	A	79	24.304	14.292	5.666	1.00	30.04	6
	ATOM	629	C	CYS	A	79	22.949	13.894	5.111	1.00	29.71	6
	ATOM	630	O	CYS	A	79	22.684	12.715	4.944	1.00	29.58	8
60	ATOM	631	CB	CYS	A	79	24.188	14.507	7.183	1.00	31.67	6
	ATOM	632	SG	CYS	A	79	25.844	14.386	7.916	1.00	33.92	16
	ATOM	633	N	GLU	A	80	22.134	14.874	4.734	1.00	30.93	7
	ATOM	634	CA	GLU	A	80	20.899	14.555	4.007	1.00	32.01	6
	ATOM	635	C	GLU	A	80	21.197	13.812	2.705	1.00	29.17	6
65	ATOM	636	O	GLU	A	80	20.524	12.822	2.413	1.00	29.08	8
	ATOM	637	CB	GLU	A	80	20.135	15.852	3.756	1.00	36.34	6
	ATOM	638	CG	GLU	A	80	19.379	16.349	4.985	1.00	43.73	6
	ATOM	639	CD	GLU	A	80	18.700	17.700	4.818	1.00	48.86	6
	ATOM	640	OE1	GLU	A	80	18.432	18.156	3.670	1.00	51.62	8
70	ATOM	641	OE2	GLU	A	80	18.442	18.338	5.884	1.00	51.33	8
	ATOM	642	N	LYS	A	81	22.175	14.264	1.921	1.00	26.79	7
	ATOM	643	CA	LYS	A	81	22.522	13.581	0.676	1.00	27.73	6
	ATOM	644	C	LYS	A	81	23.067	12.161	0.921	1.00	27.62	6
	ATOM	645	O	LYS	A	81	22.686	11.291	0.147	1.00	25.90	8
	ATOM	646	CB	LYS	A	81	23.541	14.390	-0.112	1.00	27.61	6

-45-

	ATOM	647	CG	LYS	A	81	23.036	15.708	-0.702	1.00	27.05	6
	ATOM	648	CD	LYS	A	81	24.149	16.381	-1.485	1.00	29.23	6
	ATOM	649	CE	LYS	A	81	23.586	17.726	-1.958	1.00	31.40	6
5	ATOM	650	NZ	LYS	A	81	24.290	18.189	-3.180	1.00	33.21	7
	ATOM	651	N	LEU	A	82	23.941	12.067	1.932	1.00	25.01	7
	ATOM	652	CA	LEU	A	82	24.428	10.653	2.208	1.00	25.50	6
	ATOM	653	C	LEU	A	82	23.359	9.729	2.719	1.00	24.46	6
	ATOM	654	O	LEU	A	82	23.296	8.571	2.335	1.00	25.35	8
10	ATOM	655	CB	LEU	A	82	25.616	10.767	3.179	1.00	24.87	6
	ATOM	656	CG	LEU	A	82	26.765	11.600	2.627	1.00	25.74	6
	ATOM	657	CD1	LEU	A	82	27.854	11.923	3.663	1.00	24.08	6
	ATOM	658	CD2	LEU	A	82	27.412	10.853	1.463	1.00	24.64	6
	ATOM	659	N	ASN	A	83	22.437	10.262	3.549	1.00	27.59	7
15	ATOM	660	CA	ASN	A	83	21.352	9.467	4.081	1.00	29.62	6
	ATOM	661	C	ASN	A	83	20.400	9.086	2.941	1.00	31.66	6
	ATOM	662	O	ASN	A	83	20.066	7.899	2.966	1.00	31.60	8
	ATOM	663	CB	ASN	A	83	20.649	10.212	5.205	1.00	32.77	6
	ATOM	664	CG	ASN	A	83	19.718	9.324	6.010	1.00	37.49	6
20	ATOM	665	OD1	ASN	A	83	18.788	9.898	6.588	1.00	42.54	8
	ATOM	666	ND2	ASN	A	83	19.899	8.019	6.093	1.00	37.69	7
	ATOM	667	N	LYS	A	84	20.176	9.954	1.933	1.00	31.56	7
	ATOM	668	CA	LYS	A	84	19.397	9.440	0.781	1.00	33.04	6
	ATOM	669	C	LYS	A	84	20.155	8.440	-0.069	1.00	34.14	6
25	ATOM	670	O	LYS	A	84	19.531	7.661	-0.824	1.00	34.69	8
	ATOM	671	CB	LYS	A	84	18.915	10.637	-0.071	1.00	36.71	6
	ATOM	672	CG	LYS	A	84	17.639	11.350	0.339	1.00	42.14	6
	ATOM	673	CD	LYS	A	84	17.457	12.707	-0.355	1.00	45.16	6
	ATOM	674	CE	LYS	A	84	16.334	13.494	0.303	1.00	48.19	6
30	ATOM	675	NZ	LYS	A	84	16.337	14.928	-0.105	1.00	50.51	7
	ATOM	676	N	ARG	A	85	21.483	8.305	0.021	1.00	34.32	7
	ATOM	677	CA	ARG	A	85	22.276	7.344	-0.773	1.00	33.70	6
	ATOM	678	C	ARG	A	85	22.620	6.057	-0.050	1.00	34.60	6
	ATOM	679	O	ARG	A	85	23.358	5.112	-0.377	1.00	36.33	8
35	ATOM	680	CB	ARG	A	85	23.529	8.099	-1.166	1.00	34.84	6
	ATOM	681	CG	ARG	A	85	24.040	7.946	-2.583	1.00	36.24	6
	ATOM	682	CD	ARG	A	85	23.177	8.780	-3.502	1.00	37.79	6
	ATOM	683	NE	ARG	A	85	23.549	8.555	-4.891	1.00	36.63	7
	ATOM	684	CZ	ARG	A	85	23.122	9.364	-5.853	1.00	37.76	6
40	ATOM	685	NH1	ARG	A	85	22.368	10.397	-5.507	1.00	38.88	7
	ATOM	686	NH2	ARG	A	85	23.473	9.117	-7.100	1.00	37.39	7
	ATOM	687	N	LYS	A	86	21.948	5.940	1.093	1.00	33.51	7
	ATOM	688	CA	LYS	A	86	21.983	4.881	2.059	1.00	34.48	6
	ATOM	689	C	LYS	A	86	23.404	4.563	2.503	1.00	32.25	6
45	ATOM	690	O	LYS	A	86	23.823	3.405	2.516	1.00	34.37	8
	ATOM	691	CB	LYS	A	86	21.290	3.624	1.477	1.00	37.47	6
	ATOM	692	CG	LYS	A	86	19.862	3.957	1.034	1.00	42.40	6
	ATOM	693	CD	LYS	A	86	18.990	4.373	2.205	1.00	46.88	6
	ATOM	694	CE	LYS	A	86	18.857	3.256	3.233	1.00	50.03	6
50	ATOM	695	NZ	LYS	A	86	18.397	3.827	4.543	1.00	52.47	7
	ATOM	696	N	VAL	A	87	24.138	5.595	2.885	1.00	29.97	7
	ATOM	697	CA	VAL	A	87	25.490	5.405	3.428	1.00	26.05	6
	ATOM	698	C	VAL	A	87	25.390	4.849	4.829	1.00	28.43	6
	ATOM	699	O	VAL	A	87	24.498	5.233	5.587	1.00	26.14	8
55	ATOM	700	CB	VAL	A	87	26.199	6.749	3.397	1.00	26.58	6
	ATOM	701	CG1	VAL	A	87	27.425	6.848	4.304	1.00	23.69	6
	ATOM	702	CG2	VAL	A	87	26.640	7.063	1.961	1.00	25.53	6
	ATOM	703	N	ASP	A	88	26.274	3.947	5.231	1.00	25.06	7
	ATOM	704	CA	ASP	A	88	26.163	3.320	6.552	1.00	27.11	6
60	ATOM	705	C	ASP	A	88	26.718	4.129	7.696	1.00	26.68	6
	ATOM	706	O	ASP	A	88	26.108	4.221	8.763	1.00	27.00	8
	ATOM	707	CB	ASP	A	88	26.899	1.986	6.461	1.00	29.00	6
	ATOM	708	CG	ASP	A	88	26.332	1.114	5.377	1.00	31.90	6
	ATOM	709	OD1	ASP	A	88	25.301	0.444	5.714	1.00	34.25	8
65	ATOM	710	OD2	ASP	A	88	26.819	1.060	4.237	1.00	30.16	8
	ATOM	711	N	LEU	A	89	27.798	4.864	7.483	1.00	21.05	7
	ATOM	712	CA	LEU	A	89	28.448	5.620	8.532	1.00	22.89	6
	ATOM	713	C	LEU	A	89	29.085	6.879	7.997	1.00	25.24	6
	ATOM	714	O	LEU	A	89	29.775	6.771	6.967	1.00	24.36	8
70	ATOM	715	CB	LEU	A	89	29.561	4.723	9.069	1.00	27.61	6
	ATOM	716	CG	LEU	A	89	30.275	5.099	10.342	1.00	31.35	6
	ATOM	717	CD1	LEU	A	89	30.916	3.857	10.963	1.00	34.98	6
	ATOM	718	CD2	LEU	A	89	31.363	6.137	10.099	1.00	33.01	6
	ATOM	719	N	VAL	A	90	28.910	7.987	8.677	1.00	22.49	7
	ATOM	720	CA	VAL	A	90	29.577	9.200	8.296	1.00	23.34	6

-46-

	ATOM	721	C	VAL	A	90	30.551	9.518	9.431	1.00	24.94	6
	ATOM	722	O	VAL	A	90	30.041	9.581	10.575	1.00	25.44	8
	ATOM	723	CB	VAL	A	90	28.602	10.366	8.153	1.00	21.61	6
5	ATOM	724	CG1	VAL	A	90	29.294	11.692	7.966	1.00	23.24	6
	ATOM	725	CG2	VAL	A	90	27.695	10.065	6.945	1.00	24.01	6
	ATOM	726	N	PHE	A	91	31.819	9.736	9.120	1.00	20.62	7
	ATOM	727	CA	PHE	A	91	32.779	10.106	10.131	1.00	21.25	6
	ATOM	728	C	PHE	A	91	33.008	11.589	9.966	1.00	22.65	6
10	ATOM	729	O	PHE	A	91	33.612	12.028	8.957	1.00	20.89	8
	ATOM	730	CB	PHE	A	91	34.059	9.254	9.968	1.00	20.01	6
	ATOM	731	CG	PHE	A	91	35.181	9.639	10.897	1.00	20.02	6
	ATOM	732	CD1	PHE	A	91	34.954	9.716	12.277	1.00	20.82	6
	ATOM	733	CD2	PHE	A	91	36.465	9.830	10.421	1.00	21.38	6
15	ATOM	734	CE1	PHE	A	91	36.004	10.045	13.150	1.00	21.05	6
	ATOM	735	CE2	PHE	A	91	37.503	10.196	11.281	1.00	23.76	6
	ATOM	736	CZ	PHE	A	91	37.261	10.233	12.631	1.00	21.99	6
	ATOM	737	N	ALA	A	92	32.580	12.382	10.985	1.00	23.09	7
	ATOM	738	CA	ALA	A	92	32.750	13.824	10.898	1.00	23.04	6
20	ATOM	739	C	ALA	A	92	33.406	14.387	12.142	1.00	24.15	6
	ATOM	740	O	ALA	A	92	32.699	14.986	12.979	1.00	24.45	8
	ATOM	741	CB	ALA	A	92	31.368	14.496	10.717	1.00	23.41	6
	ATOM	742	N	PRO	A	93	34.701	14.252	12.284	1.00	23.10	7
	ATOM	743	CA	PRO	A	93	35.387	14.638	13.507	1.00	21.87	6
25	ATOM	744	C	PRO	A	93	35.695	16.093	13.560	1.00	23.67	6
	ATOM	745	O	PRO	A	93	35.740	16.790	12.510	1.00	24.71	8
	ATOM	746	CB	PRO	A	93	36.687	13.798	13.426	1.00	21.94	6
	ATOM	747	CG	PRO	A	93	37.002	13.904	11.930	1.00	23.58	6
	ATOM	748	CD	PRO	A	93	35.643	13.553	11.336	1.00	21.29	6
30	ATOM	749	N	SER	A	94	35.940	16.664	14.752	1.00	23.63	7
	ATOM	750	CA	SER	A	94	36.447	18.022	14.812	1.00	26.17	6
	ATOM	751	C	SER	A	94	37.939	18.117	14.561	1.00	26.12	6
	ATOM	752	O	SER	A	94	38.700	17.126	14.588	1.00	25.24	8
	ATOM	753	CB	SER	A	94	36.151	18.617	16.207	1.00	26.90	6
35	ATOM	754	OG	SER	A	94	36.930	17.871	17.168	1.00	27.23	8
	ATOM	755	N	VAL	A	95	38.487	19.308	14.308	1.00	25.69	7
	ATOM	756	CA	VAL	A	95	39.900	19.519	14.115	1.00	25.50	6
	ATOM	757	C	VAL	A	95	40.639	19.107	15.409	1.00	28.17	6
	ATOM	758	O	VAL	A	95	41.692	18.475	15.307	1.00	27.54	8
40	ATOM	759	CB	VAL	A	95	40.319	20.963	13.788	1.00	27.40	6
	ATOM	760	CG1	VAL	A	95	41.808	21.236	13.929	1.00	27.91	6
	ATOM	761	CG2	VAL	A	95	39.873	21.263	12.346	1.00	26.36	6
	ATOM	762	N	LYS	A	96	40.047	19.405	16.570	1.00	26.82	7
	ATOM	763	CA	LYS	A	96	40.718	18.994	17.823	1.00	28.89	6
45	ATOM	764	C	LYS	A	96	40.773	17.474	17.962	1.00	28.61	6
	ATOM	765	O	LYS	A	96	41.723	16.951	18.539	1.00	27.95	8
	ATOM	766	CB	LYS	A	96	40.013	19.550	19.066	1.00	29.19	6
	ATOM	767	N	GLU	A	97	39.756	16.765	17.486	1.00	28.36	7
	ATOM	768	CA	GLU	A	97	39.748	15.295	17.583	1.00	29.80	6
50	ATOM	769	C	GLU	A	97	40.830	14.674	16.708	1.00	29.13	6
	ATOM	770	O	GLU	A	97	41.565	13.752	17.126	1.00	29.24	8
	ATOM	771	CB	GLU	A	97	38.365	14.782	17.214	1.00	29.05	6
	ATOM	772	CG	GLU	A	97	38.194	13.265	17.303	1.00	28.83	6
	ATOM	773	CD	GLU	A	97	38.133	12.796	18.762	1.00	30.81	6
55	ATOM	774	OE1	GLU	A	97	38.046	13.687	19.649	1.00	32.00	8
	ATOM	775	OE2	GLU	A	97	38.132	11.592	19.080	1.00	28.32	8
	ATOM	776	N	ILE	A	98	41.066	15.194	15.516	1.00	26.74	7
	ATOM	777	CA	ILE	A	98	42.110	14.673	14.641	1.00	24.88	6
	ATOM	778	C	ILE	A	98	43.483	15.219	14.955	1.00	26.67	6
60	ATOM	779	O	ILE	A	98	44.485	14.459	14.852	1.00	24.09	8
	ATOM	780	CB	ILE	A	98	41.817	14.972	13.147	1.00	23.79	6
	ATOM	781	CG1	ILE	A	98	40.483	14.337	12.789	1.00	22.35	6
	ATOM	782	CG2	ILE	A	98	42.971	14.486	12.252	1.00	22.39	6
	ATOM	783	CD1	ILE	A	98	40.431	12.804	12.865	1.00	24.57	6
65	ATOM	784	N	TYR	A	99	43.603	16.493	15.375	1.00	24.39	7
	ATOM	785	CA	TYR	A	99	44.886	17.127	15.585	1.00	26.57	6
	ATOM	786	C	TYR	A	99	44.917	17.788	16.978	1.00	26.98	6
	ATOM	787	O	TYR	A	99	44.959	18.984	17.080	1.00	29.92	8
	ATOM	788	CB	TYR	A	99	45.244	18.185	14.514	1.00	24.58	6
70	ATOM	789	CG	TYR	A	99	45.318	17.673	13.080	1.00	24.59	6
	ATOM	790	CD1	TYR	A	99	44.461	18.086	12.085	1.00	23.63	6
	ATOM	791	CD2	TYR	A	99	46.371	16.838	12.709	1.00	23.01	6
	ATOM	792	CE1	TYR	A	99	44.573	17.677	10.760	1.00	23.55	6
	ATOM	793	CE2	TYR	A	99	46.491	16.358	11.405	1.00	25.75	6
	ATOM	794	CZ	TYR	A	99	45.593	16.773	10.447	1.00	24.33	6

-47-

	ATOM	795	OH	TYR	A	99	45.814	16.340	9.160	1.00	22.62	8
	ATOM	796	N	PRO	A	100	44.891	17.004	18.020	1.00	29.54	7
	ATOM	797	CA	PRO	A	100	44.819	17.563	19.401	1.00	30.81	6
	ATOM	798	C	PRO	A	100	46.024	18.411	19.723	1.00	33.04	6
5	ATOM	799	O	PRO	A	100	45.855	19.351	20.545	1.00	34.95	8
	ATOM	800	CB	PRO	A	100	44.652	16.358	20.291	1.00	32.03	6
	ATOM	801	CG	PRO	A	100	45.376	15.277	19.517	1.00	31.65	6
	ATOM	802	CD	PRO	A	100	44.894	15.532	18.081	1.00	29.86	6
10	ATOM	803	N	ASN	A	101	47.177	18.234	19.116	1.00	30.09	7
	ATOM	804	CA	ASN	A	101	48.364	19.030	19.406	1.00	29.38	6
	ATOM	805	C	ASN	A	101	48.732	19.925	18.258	1.00	28.34	6
	ATOM	806	O	ASN	A	101	49.831	20.474	18.133	1.00	29.73	8
	ATOM	807	CB	ASN	A	101	49.573	18.111	19.726	1.00	32.63	6
15	ATOM	808	CG	ASN	A	101	49.136	17.044	20.693	1.00	32.29	6
	ATOM	809	OD1	ASN	A	101	49.095	15.839	20.358	1.00	35.88	8
	ATOM	810	ND2	ASN	A	101	48.725	17.480	21.868	1.00	33.54	7
	ATOM	811	N	GLY	A	102	47.764	20.158	17.344	1.00	28.24	7
	ATOM	812	CA	GLY	A	102	48.018	20.969	16.192	1.00	28.54	6
20	ATOM	813	C	GLY	A	102	48.572	20.122	15.054	1.00	28.73	6
	ATOM	814	O	GLY	A	102	48.848	18.918	15.212	1.00	28.80	8
	ATOM	815	N	THR	A	103	48.797	20.786	13.929	1.00	28.45	7
	ATOM	816	CA	THR	A	103	49.271	20.035	12.755	1.00	27.44	6
	ATOM	817	C	THR	A	103	50.751	20.121	12.584	1.00	27.75	6
25	ATOM	818	O	THR	A	103	51.419	19.270	11.979	1.00	28.24	8
	ATOM	819	CB	THR	A	103	48.585	20.545	11.461	1.00	28.39	6
	ATOM	820	OG1	THR	A	103	49.011	21.911	11.287	1.00	29.31	8
	ATOM	821	CG2	THR	A	103	47.081	20.410	11.575	1.00	25.68	6
	ATOM	822	N	GLU	A	104	51.410	21.114	13.189	1.00	26.94	7
30	ATOM	823	CA	GLU	A	104	52.843	21.274	12.953	1.00	30.65	6
	ATOM	824	C	GLU	A	104	53.682	20.149	13.572	1.00	27.87	6
	ATOM	825	O	GLU	A	104	54.755	19.902	13.010	1.00	30.98	8
	ATOM	826	CB	GLU	A	104	53.353	22.617	13.515	1.00	34.13	6
	ATOM	827	CG	GLU	A	104	52.613	23.746	12.784	1.00	40.22	6
35	ATOM	828	CD	GLU	A	104	51.319	24.211	13.411	1.00	44.21	6
	ATOM	829	OE1	GLU	A	104	50.583	23.551	14.187	1.00	42.68	8
	ATOM	830	OE2	GLU	A	104	50.972	25.409	13.090	1.00	48.99	8
	ATOM	831	N	THR	A	105	53.210	19.618	14.686	1.00	24.87	7
	ATOM	832	CA	THR	A	105	54.112	18.554	15.230	1.00	25.37	6
40	ATOM	833	C	THR	A	105	53.586	17.170	14.962	1.00	24.14	6
	ATOM	834	O	THR	A	105	54.100	16.162	15.504	1.00	23.64	8
	ATOM	835	CB	THR	A	105	54.301	18.763	16.735	1.00	24.29	6
	ATOM	836	OG1	THR	A	105	53.037	18.773	17.363	1.00	27.37	8
	ATOM	837	CG2	THR	A	105	55.020	20.098	16.999	1.00	27.01	6
45	ATOM	838	N	HIS	A	106	52.456	17.094	14.251	1.00	22.37	7
	ATOM	839	CA	HIS	A	106	51.897	15.760	13.955	1.00	22.53	6
	ATOM	840	C	HIS	A	106	52.748	15.031	12.927	1.00	20.08	6
	ATOM	841	O	HIS	A	106	53.289	15.552	11.960	1.00	22.95	8
	ATOM	842	CB	HIS	A	106	50.457	15.962	13.432	1.00	20.21	6
50	ATOM	843	CG	HIS	A	106	49.534	14.791	13.386	1.00	19.83	6
	ATOM	844	ND1	HIS	A	106	49.650	13.883	12.350	1.00	19.73	7
	ATOM	845	CD2	HIS	A	106	48.484	14.387	14.112	1.00	18.64	6
	ATOM	846	CE1	HIS	A	106	48.695	13.003	12.509	1.00	17.48	6
	ATOM	847	NE2	HIS	A	106	47.914	13.255	13.533	1.00	19.68	7
55	ATOM	848	N	THR	A	107	52.772	13.689	13.062	1.00	21.05	7
	ATOM	849	CA	THR	A	107	53.466	12.840	12.117	1.00	20.53	6
	ATOM	850	C	THR	A	107	52.946	13.066	10.697	1.00	20.02	6
	ATOM	851	O	THR	A	107	51.730	13.301	10.684	1.00	20.34	8
	ATOM	852	CB	THR	A	107	53.232	11.366	12.525	1.00	21.22	6
60	ATOM	853	OG1	THR	A	107	53.808	11.185	13.848	1.00	22.21	8
	ATOM	854	CG2	THR	A	107	53.856	10.364	11.540	1.00	21.83	6
	ATOM	855	N	TYR	A	108	53.769	13.113	9.699	1.00	20.01	7
	ATOM	856	CA	TYR	A	108	53.224	13.286	8.347	1.00	22.77	6
	ATOM	857	C	TYR	A	108	53.796	12.231	7.405	1.00	21.91	6
65	ATOM	858	O	TYR	A	108	54.794	11.532	7.605	1.00	19.88	8
	ATOM	859	CB	TYR	A	108	53.505	14.695	7.860	1.00	23.51	6
	ATOM	860	CG	TYR	A	108	54.978	15.076	7.762	1.00	24.54	6
	ATOM	861	CD1	TYR	A	108	55.707	14.832	6.624	1.00	25.82	6
	ATOM	862	CD2	TYR	A	108	55.623	15.677	8.857	1.00	26.49	6
70	ATOM	863	CE1	TYR	A	108	57.051	15.146	6.526	1.00	29.12	6
	ATOM	864	CE2	TYR	A	108	56.970	16.024	8.781	1.00	29.06	6
	ATOM	865	CZ	TYR	A	108	57.664	15.733	7.631	1.00	29.44	6
	ATOM	866	OH	TYR	A	108	58.995	16.072	7.478	1.00	32.47	8
	ATOM	867	N	VAL	A	109	53.052	12.125	6.280	1.00	19.53	7
	ATOM	868	CA	VAL	A	109	53.431	11.213	5.194	1.00	20.38	6

-48-

	ATOM	869	C	VAL	A	109	53.653	12.022	3.954	1.00	24.73	6
	ATOM	870	O	VAL	A	109	52.756	12.811	3.553	1.00	23.81	8
	ATOM	871	CB	VAL	A	109	52.263	10.230	4.964	1.00	20.04	6
5	ATOM	872	CG1	VAL	A	109	52.619	9.362	3.731	1.00	23.57	6
	ATOM	873	CG2	VAL	A	109	51.946	9.420	6.209	1.00	17.72	6
	ATOM	874	N	ASP	A	110	54.753	11.885	3.237	1.00	25.18	7
	ATOM	875	CA	ASP	A	110	55.054	12.663	2.047	1.00	28.26	6
	ATOM	876	C	ASP	A	110	55.453	11.784	0.881	1.00	25.00	6
10	ATOM	877	O	ASP	A	110	56.220	10.815	1.006	1.00	23.50	8
	ATOM	878	CB	ASP	A	110	56.199	13.596	2.383	1.00	34.46	6
	ATOM	879	CG	ASP	A	110	56.031	15.027	1.970	1.00	42.11	6
	ATOM	880	OD1	ASP	A	110	56.945	15.774	2.403	1.00	48.30	8
	ATOM	881	OD2	ASP	A	110	55.098	15.496	1.290	1.00	46.79	8
15	ATOM	882	N	VAL	A	111	54.851	11.964	-0.272	1.00	24.14	7
	ATOM	883	CA	VAL	A	111	55.111	11.236	-1.493	1.00	23.80	6
	ATOM	884	C	VAL	A	111	56.023	12.085	-2.363	1.00	24.56	6
	ATOM	885	O	VAL	A	111	55.572	13.037	-3.027	1.00	25.12	8
	ATOM	886	CB	VAL	A	111	53.771	10.929	-2.218	1.00	23.25	6
20	ATOM	887	CG1	VAL	A	111	54.020	10.068	-3.456	1.00	22.00	6
	ATOM	888	CG2	VAL	A	111	52.810	10.285	-1.246	1.00	22.35	6
	ATOM	889	N	PRO	A	112	57.278	11.687	-2.453	1.00	26.28	7
	ATOM	890	CA	PRO	A	112	58.274	12.438	-3.222	1.00	27.97	6
	ATOM	891	C	PRO	A	112	57.906	12.619	-4.650	1.00	30.72	6
25	ATOM	892	O	PRO	A	112	57.272	11.711	-5.253	1.00	30.37	8
	ATOM	893	CB	PRO	A	112	59.532	11.573	-3.106	1.00	27.29	6
	ATOM	894	CG	PRO	A	112	59.413	10.926	-1.769	1.00	27.60	6
	ATOM	895	CD	PRO	A	112	57.905	10.536	-1.762	1.00	24.64	6
	ATOM	896	N	GLY	A	113	58.211	13.800	-5.209	1.00	30.66	7
30	ATOM	897	CA	GLY	A	113	57.940	14.000	-6.614	1.00	32.72	6
	ATOM	898	C	GLY	A	113	56.543	14.464	-6.926	1.00	31.39	6
	ATOM	899	O	GLY	A	113	56.346	15.614	-7.280	1.00	30.61	8
	ATOM	900	N	LEU	A	114	55.558	13.575	-6.772	1.00	27.67	7
	ATOM	901	CA	LEU	A	114	54.192	13.922	-7.023	1.00	28.50	6
35	ATOM	902	C	LEU	A	114	53.677	15.086	-6.186	1.00	29.37	6
	ATOM	903	O	LEU	A	114	52.810	15.829	-6.657	1.00	33.05	8
	ATOM	904	CB	LEU	A	114	53.283	12.710	-6.702	1.00	29.66	6
	ATOM	905	CG	LEU	A	114	53.515	11.551	-7.669	1.00	31.75	6
	ATOM	906	CD1	LEU	A	114	52.703	10.351	-7.233	1.00	31.73	6
40	ATOM	907	CD2	LEU	A	114	53.134	11.977	-9.059	1.00	35.50	6
	ATOM	908	N	SER	A	115	54.161	15.180	-4.965	1.00	26.50	7
	ATOM	909	CA	SER	A	115	53.664	16.206	-4.063	1.00	27.52	6
	ATOM	910	C	SER	A	115	54.245	17.582	-4.400	1.00	30.00	6
	ATOM	911	O	SER	A	115	53.590	18.536	-3.932	1.00	28.18	8
45	ATOM	912	CB	SER	A	115	53.978	15.885	-2.599	1.00	25.46	6
	ATOM	913	OG	SER	A	115	55.407	15.846	-2.464	1.00	30.73	8
	ATOM	914	N	THR	A	116	55.312	17.617	-5.177	1.00	30.25	7
	ATOM	915	CA	THR	A	116	55.884	18.969	-5.426	1.00	32.64	6
	ATOM	916	C	THR	A	116	55.854	19.345	-6.870	1.00	33.28	6
50	ATOM	917	O	THR	A	116	56.516	20.337	-7.260	1.00	37.48	8
	ATOM	918	CB	THR	A	116	57.318	19.018	-4.839	1.00	31.68	6
	ATOM	919	OG1	THR	A	116	58.066	17.923	-5.419	1.00	33.81	8
	ATOM	920	CG2	THR	A	116	57.348	18.863	-3.344	1.00	30.91	6
	ATOM	921	N	MET	A	117	55.075	18.691	-7.725	1.00	34.70	7
55	ATOM	922	CA	MET	A	117	54.978	19.104	-9.116	1.00	36.76	6
	ATOM	923	C	MET	A	117	53.599	19.679	-9.408	1.00	35.12	6
	ATOM	924	O	MET	A	117	52.722	19.561	-8.569	1.00	34.04	8
	ATOM	925	CB	MET	A	117	55.258	17.952	-10.067	1.00	38.70	6
	ATOM	926	CG	MET	A	117	54.494	16.690	-9.707	1.00	41.51	6
60	ATOM	927	SD	MET	A	117	55.327	15.244	-10.403	1.00	45.13	16
	ATOM	928	CE	MET	A	117	55.643	15.848	-12.065	1.00	43.90	6
	ATOM	929	N	LEU	A	118	53.449	20.272	-10.578	1.00	35.18	7
	ATOM	930	CA	LEU	A	118	52.173	20.846	-10.995	1.00	36.73	6
	ATOM	931	C	LEU	A	118	51.570	21.660	-9.877	1.00	36.48	6
65	ATOM	932	O	LEU	A	118	52.236	22.552	-9.330	1.00	36.60	8
	ATOM	933	CB	LEU	A	118	51.252	19.706	-11.478	1.00	38.22	6
	ATOM	934	CG	LEU	A	118	51.872	18.829	-12.571	1.00	39.36	6
	ATOM	935	CD1	LEU	A	118	51.001	17.679	-13.051	1.00	41.36	6
	ATOM	936	CD2	LEU	A	118	52.194	19.710	-13.783	1.00	41.80	6
70	ATOM	937	N	GLU	A	119	50.329	21.339	-9.481	1.00	38.80	7
	ATOM	938	CA	GLU	A	119	49.645	22.049	-8.411	1.00	37.83	6
	ATOM	939	C	GLU	A	119	50.401	22.088	-7.102	1.00	38.27	6
	ATOM	940	O	GLU	A	119	50.416	23.101	-6.393	1.00	38.36	8
	ATOM	941	CB	GLU	A	119	48.255	21.394	-8.141	1.00	41.10	6
	ATOM	942	CG	GLU	A	119	47.470	22.109	-7.049	1.00	41.69	6

-49-

	ATOM	943	CD	GLU	A	119	46.082	21.559	-6.784	1.00	44.93	6
	ATOM	944	OE1	GLU	A	119	45.654	20.593	-7.453	1.00	40.85	8
	ATOM	945	OE2	GLU	A	119	45.379	22.098	-5.892	1.00	45.21	8
5	ATOM	946	N	GLY	A	120	51.165	21.031	-6.805	1.00	35.61	7
	ATOM	947	CA	GLY	A	120	51.945	20.951	-5.595	1.00	33.60	6
	ATOM	948	C	GLY	A	120	53.033	22.013	-5.540	1.00	34.42	6
	ATOM	949	O	GLY	A	120	53.390	22.405	-4.437	1.00	36.33	8
	ATOM	950	N	ALA	A	121	53.588	22.394	-6.677	1.00	35.01	7
10	ATOM	951	CA	ALA	A	121	54.622	23.437	-6.741	1.00	35.93	6
	ATOM	952	C	ALA	A	121	54.069	24.789	-6.295	1.00	39.30	6
	ATOM	953	O	ALA	A	121	54.752	25.536	-5.588	1.00	40.98	8
	ATOM	954	CB	ALA	A	121	55.189	23.547	-8.150	1.00	32.29	6
	ATOM	955	N	SER	A	122	52.818	25.124	-6.644	1.00	41.40	7
15	ATOM	956	CA	SER	A	122	52.261	26.415	-6.226	1.00	44.40	6
	ATOM	957	C	SER	A	122	51.626	26.354	-4.849	1.00	45.24	6
	ATOM	958	O	SER	A	122	51.056	27.328	-4.339	1.00	44.99	8
	ATOM	959	CB	SER	A	122	51.226	26.909	-7.241	1.00	45.02	6
	ATOM	960	OG	SER	A	122	50.178	25.972	-7.432	1.00	46.98	8
20	ATOM	961	N	ARG	A	123	51.634	25.169	-4.197	1.00	45.65	7
	ATOM	962	CA	ARG	A	123	51.045	24.991	-2.876	1.00	44.81	6
	ATOM	963	C	ARG	A	123	51.908	24.083	-2.006	1.00	44.93	6
	ATOM	964	O	ARG	A	123	51.557	22.916	-1.788	1.00	44.88	8
	ATOM	965	CB	ARG	A	123	49.631	24.419	-2.992	1.00	45.81	6
25	ATOM	966	CG	ARG	A	123	48.629	25.367	-3.630	1.00	46.85	6
	ATOM	967	CD	ARG	A	123	47.248	24.736	-3.714	1.00	50.24	6
	ATOM	968	NE	ARG	A	123	46.466	24.971	-2.504	1.00	52.21	7
	ATOM	969	CZ	ARG	A	123	45.271	24.437	-2.271	1.00	52.64	6
	ATOM	970	NH1	ARG	A	123	44.718	23.633	-3.169	1.00	52.96	7
30	ATOM	971	NH2	ARG	A	123	44.633	24.708	-1.141	1.00	53.34	7
	ATOM	972	N	PRO	A	124	52.717	24.827	-1.604	1.00	44.27	7
	ATOM	973	CA	PRO	A	124	53.669	24.219	-0.725	1.00	43.54	6
	ATOM	974	C	PRO	A	124	53.075	23.501	0.473	1.00	43.43	6
	ATOM	975	O	PRO	A	124	52.427	24.264	1.223	1.00	44.21	8
35	ATOM	976	CB	PRO	A	124	54.534	25.391	-0.224	1.00	43.61	6
	ATOM	977	CG	PRO	A	124	54.396	26.439	-1.257	1.00	44.17	6
	ATOM	978	CD	PRO	A	124	52.971	26.302	-1.746	1.00	44.92	6
	ATOM	979	N	GLY	A	125	53.248	21.897	0.840	1.00	39.19	7
	ATOM	980	CA	GLY	A	125	52.585	21.453	2.061	1.00	34.50	6
40	ATOM	981	C	GLY	A	125	51.230	20.789	1.809	1.00	32.64	6
	ATOM	982	O	GLY	A	125	50.689	20.112	2.669	1.00	32.97	8
	ATOM	983	N	HIS	A	126	50.594	21.246	0.725	1.00	29.92	7
	ATOM	984	CA	HIS	A	126	49.259	20.776	0.381	1.00	29.41	6
	ATOM	985	C	HIS	A	126	49.186	19.276	0.256	1.00	29.27	6
45	ATOM	986	O	HIS	A	126	48.500	18.637	1.071	1.00	29.29	8
	ATOM	987	CB	HIS	A	126	48.782	21.451	-0.934	1.00	29.82	6
	ATOM	988	CG	HIS	A	126	47.453	20.951	-1.417	1.00	30.87	6
	ATOM	989	ND1	HIS	A	126	46.254	21.263	-0.790	1.00	32.42	7
	ATOM	990	CD2	HIS	A	126	47.135	20.149	-2.435	1.00	30.12	6
50	ATOM	991	CE1	HIS	A	126	45.274	20.643	-1.373	1.00	30.81	6
	ATOM	992	NE2	HIS	A	126	45.765	19.970	-2.384	1.00	33.87	7
	ATOM	993	N	PHE	A	127	49.882	18.662	-0.698	1.00	25.60	7
	ATOM	994	CA	PHE	A	127	49.770	17.232	-0.922	1.00	25.14	6
	ATOM	995	C	PHE	A	127	50.320	16.367	0.221	1.00	24.25	6
55	ATOM	996	O	PHE	A	127	49.733	15.332	0.490	1.00	23.64	8
	ATOM	997	CB	PHE	A	127	50.454	16.851	-2.264	1.00	25.66	6
	ATOM	998	CG	PHE	A	127	49.518	17.250	-3.398	1.00	24.51	6
	ATOM	999	CD1	PHE	A	127	49.899	18.239	-4.302	1.00	25.76	6
	ATOM	1000	CD2	PHE	A	127	48.239	16.734	-3.509	1.00	26.77	6
60	ATOM	1001	CE1	PHE	A	127	49.026	18.618	-5.301	1.00	27.57	6
	ATOM	1002	CE2	PHE	A	127	47.381	17.086	-4.518	1.00	27.77	6
	ATOM	1003	CZ	PHE	A	127	47.749	18.072	-5.444	1.00	28.09	6
	ATOM	1004	N	ARG	A	128	51.218	16.966	1.006	1.00	24.68	7
	ATOM	1005	CA	ARG	A	128	51.645	16.377	2.261	1.00	23.44	6
65	ATOM	1006	C	ARG	A	128	50.408	16.283	3.155	1.00	21.06	6
	ATOM	1007	O	ARG	A	128	50.190	15.299	3.852	1.00	22.12	8
	ATOM	1008	CB	ARG	A	128	52.743	17.172	2.975	1.00	26.43	6
	ATOM	1009	CG	ARG	A	128	53.051	16.644	4.371	1.00	28.47	6
	ATOM	1010	CD	ARG	A	128	54.116	17.508	5.117	1.00	27.86	6
70	ATOM	1011	NE	ARG	A	128	55.345	17.336	4.336	1.00	31.98	7
	ATOM	1012	CZ	ARG	A	128	56.526	17.872	4.699	1.00	36.93	6
	ATOM	1013	NH1	ARG	A	128	56.631	18.561	5.825	1.00	34.28	7
	ATOM	1014	NH2	ARG	A	128	57.586	17.630	3.912	1.00	38.42	7
	ATOM	1015	N	GLY	A	129	49.588	17.337	3.161	1.00	21.21	7
	ATOM	1016	CA	GLY	A	129	48.391	17.274	4.018	1.00	21.01	6

-50-

	ATOM	1017	C	GLY	A	129	47.468	16.152	3.484	1.00	21.29	6
	ATOM	1018	O	GLY	A	129	46.782	15.601	4.321	1.00	21.30	8
	ATOM	1019	N	VAL	A	130	47.317	16.084	2.166	1.00	21.70	7
5	ATOM	1020	CA	VAL	A	130	46.441	15.028	1.634	1.00	21.40	6
	ATOM	1021	C	VAL	A	130	46.908	13.587	1.970	1.00	20.52	6
	ATOM	1022	O	VAL	A	130	46.140	12.807	2.542	1.00	19.78	8
	ATOM	1023	CB	VAL	A	130	46.256	15.179	0.107	1.00	22.23	6
	ATOM	1024	CG1	VAL	A	130	45.496	13.992	-0.479	1.00	22.29	6
10	ATOM	1025	CG2	VAL	A	130	45.587	16.550	-0.161	1.00	22.53	6
	ATOM	1026	N	SER	A	131	48.184	13.286	1.709	1.00	22.62	7
	ATOM	1027	CA	SER	A	131	48.669	11.951	2.032	1.00	22.39	6
	ATOM	1028	C	SER	A	131	48.617	11.685	3.541	1.00	20.26	6
	ATOM	1029	O	SER	A	131	48.328	10.545	3.924	1.00	22.14	8
15	ATOM	1030	CB	SER	A	131	50.095	11.641	1.549	1.00	22.52	6
	ATOM	1031	OG	SER	A	131	50.924	12.773	1.784	1.00	24.21	8
	ATOM	1032	N	THR	A	132	48.883	12.678	4.393	1.00	17.99	7
	ATOM	1033	CA	THR	A	132	48.785	12.419	5.812	1.00	17.46	6
	ATOM	1034	C	THR	A	132	47.375	12.119	6.296	1.00	17.48	6
20	ATOM	1035	O	THR	A	132	47.180	11.104	7.013	1.00	17.25	8
	ATOM	1036	CB	THR	A	132	49.386	13.645	6.619	1.00	17.40	6
	ATOM	1037	OG1	THR	A	132	50.726	13.812	6.145	1.00	20.91	8
	ATOM	1038	CG2	THR	A	132	49.302	13.374	8.096	1.00	18.97	6
	ATOM	1039	N	ILE	A	133	46.378	12.918	5.840	1.00	17.51	7
25	ATOM	1040	CA	ILE	A	133	45.048	12.635	6.366	1.00	17.42	6
	ATOM	1041	C	ILE	A	133	44.514	11.317	5.727	1.00	17.76	6
	ATOM	1042	O	ILE	A	133	43.831	10.598	6.432	1.00	16.73	8
	ATOM	1043	CB	ILE	A	133	44.056	13.814	6.199	1.00	19.04	6
	ATOM	1044	CG1	ILE	A	133	42.772	13.574	6.991	1.00	18.12	6
30	ATOM	1045	CG2	ILE	A	133	43.692	14.007	4.713	1.00	19.62	6
	ATOM	1046	CD1	ILE	A	133	43.077	13.562	8.543	1.00	19.23	6
	ATOM	1047	N	VAL	A	134	44.834	11.013	4.468	1.00	20.06	7
	ATOM	1048	CA	VAL	A	134	44.318	9.805	3.843	1.00	20.66	6
	ATOM	1049	C	VAL	A	134	44.943	8.567	4.523	1.00	16.68	6
35	ATOM	1050	O	VAL	A	134	44.181	7.608	4.840	1.00	16.16	8
	ATOM	1051	CB	VAL	A	134	44.556	9.769	2.329	1.00	20.12	6
	ATOM	1052	CG1	VAL	A	134	43.968	8.529	1.685	1.00	20.31	6
	ATOM	1053	CG2	VAL	A	134	43.953	11.019	1.680	1.00	21.96	6
	ATOM	1054	N	SER	A	135	46.232	8.622	4.793	1.00	17.42	7
40	ATOM	1055	CA	SER	A	135	46.862	7.515	5.554	1.00	18.57	6
	ATOM	1056	C	SER	A	135	46.167	7.337	6.870	1.00	18.10	6
	ATOM	1057	O	SER	A	135	45.906	6.226	7.307	1.00	17.58	8
	ATOM	1058	CB	SER	A	135	48.367	7.725	5.776	1.00	21.85	6
	ATOM	1059	OG	SER	A	135	49.165	7.574	4.629	1.00	26.07	8
45	ATOM	1060	N	LYS	A	136	45.960	8.454	7.642	1.00	17.06	7
	ATOM	1061	CA	LYS	A	136	45.344	8.319	8.939	1.00	16.75	6
	ATOM	1062	C	LYS	A	136	43.943	7.726	8.855	1.00	16.59	6
	ATOM	1063	O	LYS	A	136	43.549	6.804	9.565	1.00	17.77	8
	ATOM	1064	CB	LYS	A	136	45.347	9.698	9.654	1.00	17.50	6
50	ATOM	1065	CG	LYS	A	136	44.778	9.658	11.055	1.00	17.92	6
	ATOM	1066	CD	LYS	A	136	45.193	10.949	11.821	1.00	18.19	6
	ATOM	1067	CE	LYS	A	136	44.719	10.824	13.255	1.00	20.47	6
	ATOM	1068	NZ	LYS	A	136	45.341	11.921	14.099	1.00	21.74	7
	ATOM	1069	N	LEU	A	137	43.114	8.215	7.905	1.00	16.58	7
55	ATOM	1070	CA	LEU	A	137	41.820	7.610	7.620	1.00	16.97	6
	ATOM	1071	C	LEU	A	137	41.917	6.145	7.208	1.00	16.87	6
	ATOM	1072	O	LEU	A	137	41.086	5.366	7.671	1.00	18.31	8
	ATOM	1073	CB	LEU	A	137	41.186	8.426	6.450	1.00	16.26	6
	ATOM	1074	CG	LEU	A	137	40.680	9.774	6.970	1.00	19.05	6
60	ATOM	1075	CD1	LEU	A	137	40.287	10.582	5.686	1.00	19.51	6
	ATOM	1076	CD2	LEU	A	137	39.540	9.723	7.939	1.00	20.72	6
	ATOM	1077	N	PHE	A	138	42.967	5.788	6.451	1.00	16.58	7
	ATOM	1078	CA	PHE	A	138	43.010	4.341	6.127	1.00	18.39	6
	ATOM	1079	C	PHE	A	138	43.255	3.486	7.348	1.00	18.60	6
65	ATOM	1080	O	PHE	A	138	42.757	2.384	7.504	1.00	17.30	8
	ATOM	1081	CB	PHE	A	138	44.122	4.115	5.093	1.00	17.12	6
	ATOM	1082	CG	PHE	A	138	43.764	4.570	3.689	1.00	18.73	6
	ATOM	1083	CD1	PHE	A	138	44.806	4.543	2.766	1.00	17.88	6
	ATOM	1084	CD2	PHE	A	138	42.473	4.892	3.307	1.00	18.91	6
70	ATOM	1085	CE1	PHE	A	138	44.536	4.879	1.448	1.00	20.01	6
	ATOM	1086	CE2	PHE	A	138	42.230	5.257	1.997	1.00	19.56	6
	ATOM	1087	CZ	PHE	A	138	43.254	5.215	1.074	1.00	19.96	6
	ATOM	1088	N	ASN	A	139	44.082	4.007	8.264	1.00	18.42	7
	ATOM	1089	CA	ASN	A	139	44.379	3.252	9.498	1.00	18.84	6
	ATOM	1090	C	ASN	A	139	43.214	3.179	10.420	1.00	18.89	6

-51-

	ATOM	1091	O	ASN	A	139	43.006	2.188	11.154	1.00	20.77	8
	ATOM	1092	CB	ASN	A	139	45.584	3.896	10.226	1.00	18.65	6
	ATOM	1093	CG	ASN	A	139	46.893	3.695	9.486	1.00	21.58	6
5	ATOM	1094	OD1	ASN	A	139	47.077	2.678	8.835	1.00	23.27	8
	ATOM	1095	ND2	ASN	A	139	47.838	4.616	9.605	1.00	23.11	7
	ATOM	1096	N	LEU	A	140	42.380	4.245	10.477	1.00	18.73	7
	ATOM	1097	CA	LEU	A	140	41.227	4.287	11.337	1.00	19.89	6
	ATOM	1098	C	LEU	A	140	40.035	3.500	10.798	1.00	22.66	6
10	ATOM	1099	O	LEU	A	140	39.348	2.886	11.581	1.00	23.40	8
	ATOM	1100	CB	LEU	A	140	40.725	5.736	11.530	1.00	19.74	6
	ATOM	1101	CG	LEU	A	140	41.667	6.734	12.211	1.00	20.69	6
	ATOM	1102	CD1	LEU	A	140	41.159	8.189	12.222	1.00	20.47	6
	ATOM	1103	CD2	LEU	A	140	41.923	6.357	13.687	1.00	21.82	6
15	ATOM	1104	N	VAL	A	141	39.777	3.644	9.493	1.00	21.89	7
	ATOM	1105	CA	VAL	A	141	38.625	2.951	8.912	1.00	18.58	6
	ATOM	1106	C	VAL	A	141	38.930	1.566	8.477	1.00	18.27	6
	ATOM	1107	O	VAL	A	141	37.992	0.726	8.348	1.00	21.83	8
	ATOM	1108	CB	VAL	A	141	38.121	3.897	7.749	1.00	17.89	6
20	ATOM	1109	CG1	VAL	A	141	37.004	3.204	6.948	1.00	19.45	6
	ATOM	1110	CG2	VAL	A	141	37.684	5.229	8.360	1.00	19.31	6
	ATOM	1111	N	GLN	A	142	40.157	1.207	8.147	1.00	19.32	7
	ATOM	1112	CA	GLN	A	142	40.614	-0.046	7.611	1.00	22.31	6
	ATOM	1113	C	GLN	A	142	39.731	-0.535	6.460	1.00	19.60	6
25	ATOM	1114	O	GLN	A	142	39.182	-1.647	6.518	1.00	20.68	8
	ATOM	1115	CB	GLN	A	142	40.661	-1.162	8.674	1.00	23.95	6
	ATOM	1116	CG	GLN	A	142	41.594	-0.685	9.829	1.00	28.73	6
	ATOM	1117	CD	GLN	A	142	41.536	-1.705	10.951	1.00	34.39	6
	ATOM	1118	OE1	GLN	A	142	42.491	-2.469	11.021	1.00	39.24	8
30	ATOM	1119	NE2	GLN	A	142	40.502	-1.784	11.754	1.00	35.26	7
	ATOM	1120	N	PRO	A	143	39.558	0.297	5.442	1.00	18.88	7
	ATOM	1121	CA	PRO	A	143	38.717	-0.119	4.346	1.00	18.57	6
	ATOM	1122	C	PRO	A	143	39.398	-1.140	3.497	1.00	19.27	6
	ATOM	1123	O	PRO	A	143	40.627	-1.225	3.382	1.00	21.22	8
35	ATOM	1124	CB	PRO	A	143	38.538	1.179	3.558	1.00	17.81	6
	ATOM	1125	CG	PRO	A	143	39.829	1.905	3.755	1.00	17.73	6
	ATOM	1126	CD	PRO	A	143	40.201	1.627	5.230	1.00	17.54	6
	ATOM	1127	N	ASP	A	144	38.648	-1.982	2.768	1.00	17.55	7
	ATOM	1128	CA	ASP	A	144	39.097	-2.852	1.720	1.00	20.28	6
40	ATOM	1129	C	ASP	A	144	39.283	-2.125	0.399	1.00	19.25	6
	ATOM	1130	O	ASP	A	144	40.083	-2.459	-0.481	1.00	20.98	8
	ATOM	1131	CB	ASP	A	144	38.033	-3.936	1.546	1.00	20.76	6
	ATOM	1132	CG	ASP	A	144	37.957	-4.815	2.798	1.00	26.72	6
	ATOM	1133	OD1	ASP	A	144	36.961	-4.629	3.528	1.00	28.28	8
45	ATOM	1134	OD2	ASP	A	144	38.895	-5.587	3.031	1.00	31.50	8
	ATOM	1135	N	ILE	A	145	38.477	-1.081	0.131	1.00	17.25	7
	ATOM	1136	CA	ILE	A	145	38.375	-0.260	-1.035	1.00	18.60	6
	ATOM	1137	C	ILE	A	145	38.239	1.190	-0.687	1.00	18.09	6
	ATOM	1138	O	ILE	A	145	37.607	1.491	0.327	1.00	18.47	8
50	ATOM	1139	CB	ILE	A	145	37.081	-0.719	-1.802	1.00	22.13	6
	ATOM	1140	CG1	ILE	A	145	37.350	-2.164	-2.291	1.00	26.63	6
	ATOM	1141	CG2	ILE	A	145	36.613	0.193	-2.934	1.00	28.58	6
	ATOM	1142	CD1	ILE	A	145	35.987	-2.820	-2.537	1.00	33.01	6
	ATOM	1143	N	ALA	A	146	38.745	2.119	-1.471	1.00	18.54	7
55	ATOM	1144	CA	ALA	A	146	38.555	3.525	-1.287	1.00	17.65	6
	ATOM	1145	C	ALA	A	146	38.386	4.174	-2.669	1.00	18.82	6
	ATOM	1146	O	ALA	A	146	39.158	3.831	-3.590	1.00	20.86	8
	ATOM	1147	CB	ALA	A	146	39.754	4.169	-0.561	1.00	17.02	6
	ATOM	1148	N	CYS	A	147	37.421	5.032	-2.758	1.00	17.39	7
60	ATOM	1149	CA	CYS	A	147	37.059	5.669	-4.042	1.00	19.79	6
	ATOM	1150	C	CYS	A	147	37.462	7.132	-4.108	1.00	20.20	6
	ATOM	1151	O	CYS	A	147	37.292	7.934	-3.181	1.00	20.69	8
	ATOM	1152	CB	CYS	A	147	35.534	5.576	-4.235	1.00	21.84	6
	ATOM	1153	SG	CYS	A	147	34.881	3.895	-4.275	1.00	25.91	16
65	ATOM	1154	N	PHE	A	148	38.073	7.481	-5.256	1.00	20.78	7
	ATOM	1155	CA	PHE	A	148	38.521	8.824	-5.534	1.00	20.56	6
	ATOM	1156	C	PHE	A	148	38.105	9.201	-6.955	1.00	20.31	6
	ATOM	1157	O	PHE	A	148	38.047	8.291	-7.790	1.00	21.33	8
	ATOM	1158	CB	PHE	A	148	40.044	8.856	-5.392	1.00	19.98	6
70	ATOM	1159	CG	PHE	A	148	40.527	8.697	-3.964	1.00	21.76	6
	ATOM	1160	CD1	PHE	A	148	40.803	7.418	-3.472	1.00	21.62	6
	ATOM	1161	CD2	PHE	A	148	40.682	9.781	-3.137	1.00	24.08	6
	ATOM	1162	CE1	PHE	A	148	41.217	7.237	-2.164	1.00	21.64	6
	ATOM	1163	CE2	PHE	A	148	41.150	9.580	-1.833	1.00	22.23	6
	ATOM	1164	CZ	PHE	A	148	41.384	8.321	-1.337	1.00	21.48	6

-52-

	ATOM	1165	N	GLY	A	149	37.874	10.485	-7.215	1.00	19.66	7
	ATOM	1166	CA	GLY	A	149	37.457	10.782	-8.630	1.00	19.28	6
	ATOM	1167	C	GLY	A	149	38.663	10.981	-9.537	1.00	21.16	6
5	ATOM	1168	O	GLY	A	149	39.696	11.548	-9.117	1.00	25.03	8
	ATOM	1169	N	GLU	A	150	38.524	10.707	-10.848	1.00	21.70	7
	ATOM	1170	CA	GLU	A	150	39.588	10.939	-11.809	1.00	25.98	6
	ATOM	1171	C	GLU	A	150	39.777	12.386	-12.160	1.00	25.10	6
	ATOM	1172	O	GLU	A	150	40.841	12.764	-12.668	1.00	26.55	8
10	ATOM	1173	CB	GLU	A	150	39.316	10.178	-13.146	1.00	28.34	6
	ATOM	1174	CG	GLU	A	150	39.447	8.683	-12.924	1.00	30.38	6
	ATOM	1175	CD	GLU	A	150	39.464	7.923	-14.241	1.00	36.75	6
	ATOM	1176	OE1	GLU	A	150	39.222	8.536	-15.309	1.00	39.43	8
	ATOM	1177	OE2	GLU	A	150	39.770	6.715	-14.171	1.00	39.37	8
15	ATOM	1178	N	LYS	A	151	38.795	13.240	-11.874	1.00	25.17	7
	ATOM	1179	CA	LYS	A	151	38.970	14.660	-12.162	1.00	28.17	6
	ATOM	1180	C	LYS	A	151	40.159	15.229	-11.400	1.00	29.47	6
	ATOM	1181	O	LYS	A	151	40.955	16.017	-11.930	1.00	29.69	8
	ATOM	1182	CB	LYS	A	151	37.710	15.423	-11.787	1.00	30.49	6
20	ATOM	1183	CG	LYS	A	151	37.865	16.877	-12.255	1.00	34.63	6
	ATOM	1184	CD	LYS	A	151	37.021	17.827	-11.434	1.00	40.81	6
	ATOM	1185	CE	LYS	A	151	37.161	19.249	-12.007	1.00	42.71	6
	ATOM	1186	NZ	LYS	A	151	35.905	20.032	-11.825	1.00	46.87	7
	ATOM	1187	N	ASP	A	152	40.274	14.877	-10.114	1.00	26.84	7
25	ATOM	1188	CA	ASP	A	152	41.456	15.268	-9.322	1.00	26.83	6
	ATOM	1189	C	ASP	A	152	42.545	14.241	-9.529	1.00	26.30	6
	ATOM	1190	O	ASP	A	152	42.933	13.366	-8.715	1.00	24.28	8
	ATOM	1191	CB	ASP	A	152	41.078	15.419	-7.846	1.00	29.39	6
	ATOM	1192	N	PHE	A	153	43.137	14.340	-10.746	1.00	24.76	7
30	ATOM	1193	CA	PHE	A	153	44.063	13.342	-11.241	1.00	24.28	6
	ATOM	1194	C	PHE	A	153	45.350	13.353	-10.435	1.00	24.40	6
	ATOM	1195	O	PHE	A	153	45.891	12.270	-10.274	1.00	24.91	8
	ATOM	1196	CB	PHE	A	153	44.385	13.509	-12.748	1.00	26.30	6
	ATOM	1197	CG	PHE	A	153	45.137	14.809	-12.939	1.00	29.67	6
35	ATOM	1198	CD1	PHE	A	153	46.517	14.828	-13.025	1.00	30.48	6
	ATOM	1199	CD2	PHE	A	153	44.443	16.015	-13.033	1.00	32.69	6
	ATOM	1200	CE1	PHE	A	153	47.203	16.017	-13.147	1.00	31.59	6
	ATOM	1201	CE2	PHE	A	153	45.124	17.212	-13.186	1.00	33.09	6
	ATOM	1202	CZ	PHE	A	153	46.511	17.215	-13.241	1.00	34.20	6
40	ATOM	1203	N	GLN	A	154	45.781	14.510	-9.931	1.00	25.98	7
	ATOM	1204	CA	GLN	A	154	47.028	14.521	-9.174	1.00	22.85	6
	ATOM	1205	C	GLN	A	154	46.851	13.825	-7.837	1.00	22.38	6
	ATOM	1206	O	GLN	A	154	47.695	13.032	-7.413	1.00	22.53	8
	ATOM	1207	CB	GLN	A	154	47.542	15.952	-8.933	1.00	24.08	6
45	ATOM	1208	CG	GLN	A	154	48.929	15.967	-8.287	1.00	26.39	6
	ATOM	1209	CD	GLN	A	154	49.688	17.287	-8.508	1.00	28.37	6
	ATOM	1210	OE1	GLN	A	154	49.098	18.244	-8.993	1.00	28.49	8
	ATOM	1211	NE2	GLN	A	154	50.978	17.318	-8.158	1.00	26.87	7
	ATOM	1212	N	GLN	A	155	45.747	14.096	-7.174	1.00	21.22	7
50	ATOM	1213	CA	GLN	A	155	45.470	13.411	-5.896	1.00	21.76	6
	ATOM	1214	C	GLN	A	155	45.362	11.902	-6.092	1.00	21.39	6
	ATOM	1215	O	GLN	A	155	45.852	11.100	-5.289	1.00	20.96	8
	ATOM	1216	CB	GLN	A	155	44.157	13.885	-5.251	1.00	23.33	6
	ATOM	1217	CG	GLN	A	155	44.285	15.020	-4.241	0.50	22.16	6
55	ATOM	1218	CD	GLN	A	155	43.185	14.991	-3.184	0.50	22.84	6
	ATOM	1219	OE1	GLN	A	155	42.574	13.952	-2.872	0.50	25.23	8
	ATOM	1220	NE2	GLN	A	155	42.921	16.140	-2.600	0.50	20.85	7
	ATOM	1221	N	LEU	A	156	44.752	11.455	-7.214	1.00	20.25	7
	ATOM	1222	CA	LEU	A	156	44.592	10.045	-7.465	1.00	18.93	6
60	ATOM	1223	C	LEU	A	156	45.938	9.367	-7.681	1.00	20.91	6
	ATOM	1224	O	LEU	A	156	46.240	8.334	-7.081	1.00	20.99	8
	ATOM	1225	CB	LEU	A	156	43.684	9.840	-8.695	1.00	20.06	6
	ATOM	1226	CG	LEU	A	156	43.409	8.396	-9.060	1.00	21.79	6
	ATOM	1227	CD1	LEU	A	156	42.773	7.624	-7.893	1.00	20.19	6
65	ATOM	1228	CD2	LEU	A	156	42.493	8.367	-10.300	1.00	23.41	6
	ATOM	1229	N	ALA	A	157	46.790	9.991	-8.498	1.00	21.27	7
	ATOM	1230	CA	ALA	A	157	48.139	9.424	-8.654	1.00	20.85	6
	ATOM	1231	C	ALA	A	157	48.896	9.402	-7.339	1.00	22.15	6
	ATOM	1232	O	ALA	A	157	49.617	8.451	-7.039	1.00	23.09	8
70	ATOM	1233	CB	ALA	A	157	48.919	10.292	-9.658	1.00	21.65	6
	ATOM	1234	N	LEU	A	158	48.771	10.447	-6.537	1.00	21.63	7
	ATOM	1235	CA	LEU	A	158	49.507	10.508	-5.235	1.00	20.79	6
	ATOM	1236	C	LEU	A	158	49.117	9.373	-4.311	1.00	22.51	6
	ATOM	1237	O	LEU	A	158	49.950	8.663	-3.702	1.00	22.35	8
	ATOM	1238	CB	LEU	A	158	49.227	11.847	-4.583	1.00	23.18	6

-53-

	ATOM	1239	CG	LEU	A	158	49.828	12.175	-3.211	1.00	25.19	6
	ATOM	1240	CD1	LEU	A	158	51.099	12.952	-3.381	1.00	28.19	6
	ATOM	1241	CD2	LEU	A	158	48.782	12.989	-2.433	1.00	26.28	6
	ATOM	1242	N	ILE	A	159	47.765	9.231	-4.212	1.00	18.01	7
5	ATOM	1243	CA	ILE	A	159	47.322	8.127	-3.317	1.00	19.99	6
	ATOM	1244	C	ILE	A	159	47.680	6.760	-3.864	1.00	18.66	6
	ATOM	1245	O	ILE	A	159	48.038	5.871	-3.083	1.00	19.24	8
	ATOM	1246	CB	ILE	A	159	45.805	8.275	-3.083	1.00	23.08	6
10	ATOM	1247	CG1	ILE	A	159	45.455	9.626	-2.443	1.00	21.73	6
	ATOM	1248	CG2	ILE	A	159	45.232	7.181	-2.187	1.00	23.20	6
	ATOM	1249	CD1	ILE	A	159	46.056	9.774	-1.063	1.00	27.28	6
	ATOM	1250	N	ARG	A	160	47.514	6.493	-5.148	1.00	20.78	7
	ATOM	1251	CA	ARG	A	160	47.956	5.202	-5.694	1.00	20.24	6
	ATOM	1252	C	ARG	A	160	49.422	4.914	-5.397	1.00	21.57	6
15	ATOM	1253	O	ARG	A	160	49.738	3.802	-4.971	1.00	19.80	8
	ATOM	1254	CB	ARG	A	160	47.708	5.074	-7.218	1.00	21.86	6
	ATOM	1255	CG	ARG	A	160	46.192	5.007	-7.567	1.00	21.60	6
	ATOM	1256	CD	ARG	A	160	46.195	4.575	-9.066	1.00	25.76	6
20	ATOM	1257	NE	ARG	A	160	44.867	4.625	-9.678	1.00	29.84	7
	ATOM	1258	CZ	ARG	A	160	43.905	3.713	-9.455	1.00	32.53	6
	ATOM	1259	NH1	ARG	A	160	44.040	2.653	-8.651	1.00	32.58	7
	ATOM	1260	NH2	ARG	A	160	42.788	3.911	-10.168	1.00	34.80	7
	ATOM	1261	N	LYS	A	161	50.322	5.905	-5.460	1.00	20.74	7
25	ATOM	1262	CA	LYS	A	161	51.733	5.714	-5.164	1.00	19.39	6
	ATOM	1263	C	LYS	A	161	51.925	5.506	-3.674	1.00	19.31	6
	ATOM	1264	O	LYS	A	161	52.628	4.596	-3.191	1.00	22.15	8
	ATOM	1265	CB	LYS	A	161	52.523	6.929	-5.649	1.00	21.10	6
	ATOM	1266	CG	LYS	A	161	54.009	6.900	-5.202	1.00	24.79	6
30	ATOM	1267	CD	LYS	A	161	54.612	5.615	-5.820	1.00	28.31	6
	ATOM	1268	CE	LYS	A	161	56.100	5.758	-6.162	1.00	31.56	6
	ATOM	1269	NZ	LYS	A	161	56.913	6.424	-5.128	1.00	26.44	7
	ATOM	1270	N	MET	A	162	51.191	6.312	-2.834	1.00	20.30	7
	ATOM	1271	CA	MET	A	162	51.287	6.115	-1.383	1.00	18.85	6
35	ATOM	1272	C	MET	A	162	50.851	4.750	-0.908	1.00	21.35	6
	ATOM	1273	O	MET	A	162	51.504	4.085	-0.089	1.00	20.93	8
	ATOM	1274	CB	MET	A	162	50.412	7.231	-0.702	1.00	21.14	6
	ATOM	1275	CG	MET	A	162	50.512	7.132	0.818	1.00	21.47	6
	ATOM	1276	SD	MET	A	162	49.291	8.186	1.642	1.00	23.59	16
40	ATOM	1277	CE	MET	A	162	47.948	6.994	1.780	1.00	27.52	6
	ATOM	1278	N	VAL	A	163	49.808	4.217	-1.577	1.00	19.66	7
	ATOM	1279	CA	VAL	A	163	49.304	2.897	-1.214	1.00	20.50	6
	ATOM	1280	C	VAL	A	163	50.289	1.806	-1.612	1.00	19.37	6
	ATOM	1281	O	VAL	A	163	50.554	0.867	-0.837	1.00	20.07	8
45	ATOM	1282	CB	VAL	A	163	47.914	2.672	-1.873	1.00	21.79	6
	ATOM	1283	CG1	VAL	A	163	47.540	1.204	-1.894	1.00	22.15	6
	ATOM	1284	CG2	VAL	A	163	46.897	3.536	-1.100	1.00	22.77	6
	ATOM	1285	N	ALA	A	164	50.784	1.931	-2.837	1.00	21.03	7
	ATOM	1286	CA	ALA	A	164	51.773	0.937	-3.276	1.00	22.98	6
50	ATOM	1287	C	ALA	A	164	53.006	0.925	-2.380	1.00	23.44	6
	ATOM	1288	O	ALA	A	164	53.478	-0.126	-1.927	1.00	23.96	8
	ATOM	1289	CB	ALA	A	164	52.136	1.263	-4.719	1.00	23.95	6
	ATOM	1290	N	ASP	A	165	53.552	2.121	-2.154	1.00	21.54	7
	ATOM	1291	CA	ASP	A	165	54.788	2.231	-1.387	1.00	23.74	6
55	ATOM	1292	C	ASP	A	165	54.639	1.784	0.052	1.00	24.26	6
	ATOM	1293	O	ASP	A	165	55.440	1.000	0.544	1.00	24.84	8
	ATOM	1294	CB	ASP	A	165	55.321	3.664	-1.384	1.00	22.61	6
	ATOM	1295	CG	ASP	A	165	55.980	4.130	-2.662	1.00	24.69	6
	ATOM	1296	OD1	ASP	A	165	56.269	3.286	-3.531	1.00	24.19	8
60	ATOM	1297	OD2	ASP	A	165	56.220	5.356	-2.781	1.00	24.88	8
	ATOM	1298	N	MET	A	166	53.590	2.288	0.725	1.00	21.43	7
	ATOM	1299	CA	MET	A	166	53.378	2.007	2.157	1.00	20.10	6
	ATOM	1300	C	MET	A	166	52.785	0.652	2.486	1.00	21.04	6
	ATOM	1301	O	MET	A	166	52.605	0.347	3.671	1.00	21.28	8
65	ATOM	1302	CB	MET	A	166	52.540	3.142	2.751	1.00	20.75	6
	ATOM	1303	CG	MET	A	166	53.288	4.458	2.868	1.00	22.14	6
	ATOM	1304	SD	MET	A	166	55.034	4.259	3.242	1.00	26.84	16
	ATOM	1305	CE	MET	A	166	54.959	3.835	4.983	1.00	27.47	6
	ATOM	1306	N	GLY	A	167	52.458	-0.170	1.510	1.00	20.03	7
70	ATOM	1307	CA	GLY	A	167	51.975	-1.522	1.790	1.00	22.00	6
	ATOM	1308	C	GLY	A	167	50.526	-1.606	2.218	1.00	20.49	6
	ATOM	1309	O	GLY	A	167	50.190	-2.660	2.782	1.00	24.46	8
	ATOM	1310	N	PHE	A	168	49.685	-0.585	2.002	1.00	21.54	7
	ATOM	1311	CA	PHE	A	168	48.287	-0.824	2.403	1.00	20.47	6
	ATOM	1312	C	PHE	A	168	47.645	-1.917	1.546	1.00	19.05	6

-54-

	ATOM	1313	O	PHE	A	168	47.704	-1.739	0.320	1.00	20.71	8
	ATOM	1314	CB	PHE	A	168	47.563	0.509	2.296	1.00	21.24	6
	ATOM	1315	CG	PHE	A	168	47.788	1.632	3.277	1.00	20.78	6
5	ATOM	1316	CD1	PHE	A	168	48.548	2.751	2.932	1.00	22.23	6
	ATOM	1317	CD2	PHE	A	168	47.186	1.509	4.509	1.00	21.78	6
	ATOM	1318	CE1	PHE	A	168	48.736	3.747	3.913	1.00	20.66	6
	ATOM	1319	CE2	PHE	A	168	47.353	2.544	5.432	1.00	19.66	6
	ATOM	1320	CZ	PHE	A	168	48.085	3.665	5.136	1.00	20.15	6
10	ATOM	1321	N	ASP	A	169	46.769	-2.693	2.126	1.00	22.42	7
	ATOM	1322	CA	ASP	A	169	46.084	-3.767	1.356	1.00	22.89	6
	ATOM	1323	C	ASP	A	169	44.743	-3.167	0.938	1.00	23.53	6
	ATOM	1324	O	ASP	A	169	43.705	-3.617	1.427	1.00	23.13	8
	ATOM	1325	CB	ASP	A	169	45.975	-5.057	2.147	1.00	28.05	6
15	ATOM	1326	CG	ASP	A	169	45.399	-6.229	1.376	1.00	32.61	6
	ATOM	1327	OD1	ASP	A	169	45.492	-6.192	0.129	1.00	35.09	8
	ATOM	1328	OD2	ASP	A	169	44.838	-7.159	1.975	1.00	37.69	8
	ATOM	1329	N	ILE	A	170	44.751	-2.104	0.146	1.00	21.02	7
	ATOM	1330	CA	ILE	A	170	43.499	-1.409	-0.181	1.00	21.69	6
20	ATOM	1331	C	ILE	A	170	43.372	-1.265	-1.677	1.00	21.49	6
	ATOM	1332	O	ILE	A	170	44.334	-0.773	-2.304	1.00	22.63	8
	ATOM	1333	CB	ILE	A	170	43.443	-0.013	0.493	1.00	21.71	6
	ATOM	1334	CG1	ILE	A	170	43.459	-0.124	2.030	1.00	21.39	6
	ATOM	1335	CG2	ILE	A	170	42.221	0.770	0.037	1.00	22.28	6
25	ATOM	1336	CD1	ILE	A	170	43.745	1.240	2.694	1.00	23.40	6
	ATOM	1337	N	GLU	A	171	42.206	-1.583	-2.244	1.00	22.35	7
	ATOM	1338	CA	GLU	A	171	41.960	-1.346	-3.656	1.00	22.51	6
	ATOM	1339	C	GLU	A	171	41.609	0.133	-3.871	1.00	22.05	6
	ATOM	1340	O	GLU	A	171	40.625	0.577	-3.278	1.00	20.97	8
30	ATOM	1341	CB	GLU	A	171	40.841	-2.288	-4.152	1.00	21.82	6
	ATOM	1342	CG	GLU	A	171	40.514	-1.978	-5.601	1.00	28.71	6
	ATOM	1343	CD	GLU	A	171	39.364	-2.857	-6.098	1.00	34.21	6
	ATOM	1344	OE1	GLU	A	171	38.911	-3.740	-5.361	1.00	36.00	8
	ATOM	1345	OE2	GLU	A	171	38.953	-2.650	-7.272	1.00	38.31	8
35	ATOM	1346	N	ILE	A	172	42.352	0.886	-4.680	1.00	20.37	7
	ATOM	1347	CA	ILE	A	172	42.017	2.294	-4.940	1.00	19.10	6
	ATOM	1348	C	ILE	A	172	41.196	2.347	-6.217	1.00	23.26	6
	ATOM	1349	O	ILE	A	172	41.716	1.875	-7.239	1.00	26.08	8
	ATOM	1350	CB	ILE	A	172	43.306	3.159	-5.019	1.00	22.26	6
40	ATOM	1351	CG1	ILE	A	172	44.060	2.969	-3.686	1.00	21.42	6
	ATOM	1352	CG2	ILE	A	172	42.975	4.587	-5.345	1.00	23.49	6
	ATOM	1353	CD1	ILE	A	172	43.283	3.498	-2.483	1.00	22.09	6
	ATOM	1354	N	VAL	A	173	39.937	2.751	-6.114	1.00	20.87	7
	ATOM	1355	CA	VAL	A	173	39.045	2.789	-7.278	1.00	23.09	6
45	ATOM	1356	C	VAL	A	173	39.073	4.218	-7.811	1.00	23.54	6
	ATOM	1357	O	VAL	A	173	38.637	5.125	-7.058	1.00	23.05	8
	ATOM	1358	CB	VAL	A	173	37.637	2.318	-6.861	1.00	22.84	6
	ATOM	1359	CG1	VAL	A	173	36.675	2.449	-8.040	1.00	24.23	6
	ATOM	1360	CG2	VAL	A	173	37.756	0.893	-6.307	1.00	23.19	6
50	ATOM	1361	N	GLY	A	174	39.480	4.451	-9.055	1.00	22.79	7
	ATOM	1362	CA	GLY	A	174	39.509	5.765	-9.652	1.00	22.28	6
	ATOM	1363	C	GLY	A	174	38.217	5.872	-10.462	1.00	25.76	6
	ATOM	1364	O	GLY	A	174	37.972	4.984	-11.306	1.00	25.34	8
	ATOM	1365	N	VAL	A	175	37.340	6.803	-10.087	1.00	22.69	7
55	ATOM	1366	CA	VAL	A	175	35.996	6.810	-10.712	1.00	21.96	6
	ATOM	1367	C	VAL	A	175	36.025	7.779	-11.858	1.00	22.74	6
	ATOM	1368	O	VAL	A	175	36.298	8.938	-11.632	1.00	19.20	8
	ATOM	1369	CB	VAL	A	175	34.977	7.161	-9.632	1.00	21.95	6
	ATOM	1370	CG1	VAL	A	175	33.557	7.328	-10.233	1.00	23.84	6
60	ATOM	1371	CG2	VAL	A	175	34.914	6.111	-8.501	1.00	20.67	6
	ATOM	1372	N	PRO	A	176	35.590	7.430	-13.068	1.00	23.97	7
	ATOM	1373	CA	PRO	A	176	35.714	8.344	-14.172	1.00	26.00	6
	ATOM	1374	C	PRO	A	176	34.750	9.485	-14.090	1.00	23.25	6
	ATOM	1375	O	PRO	A	176	33.689	9.357	-13.462	1.00	23.13	8
65	ATOM	1376	CB	PRO	A	176	35.429	7.464	-15.401	1.00	26.90	6
	ATOM	1377	CG	PRO	A	176	35.554	6.062	-14.946	1.00	30.42	6
	ATOM	1378	CD	PRO	A	176	35.214	6.053	-13.467	1.00	26.21	6
	ATOM	1379	N	ILE	A	177	35.026	10.601	-14.706	1.00	25.15	7
	ATOM	1380	CA	ILE	A	177	34.220	11.792	-14.882	1.00	25.60	6
70	ATOM	1381	C	ILE	A	177	32.858	11.452	-15.470	1.00	26.15	6
	ATOM	1382	O	ILE	A	177	32.823	10.610	-16.392	1.00	25.13	8
	ATOM	1383	CB	ILE	A	177	35.002	12.755	-15.816	1.00	27.16	6
	ATOM	1384	CG1	ILE	A	177	36.095	13.432	-14.910	1.00	32.12	6
	ATOM	1385	CG2	ILE	A	177	34.203	13.794	-16.565	1.00	27.48	6
	ATOM	1386	CD1	ILE	A	177	37.253	13.907	-15.774	1.00	33.86	6

-55-

	ATOM	1387	N	MET	A	178	31.789	11.892	-14.839	1.00	23.56	7
	ATOM	1388	CA	MET	A	178	30.439	11.695	-15.338	1.00	22.41	6
	ATOM	1389	C	MET	A	178	30.253	12.624	-16.564	1.00	19.13	6
5	ATOM	1390	O	MET	A	178	30.623	13.780	-16.493	1.00	19.54	8
	ATOM	1391	CB	MET	A	178	29.352	12.079	-14.359	1.00	28.06	6
	ATOM	1392	CG	MET	A	178	29.443	11.331	-13.018	1.00	34.50	6
	ATOM	1393	SD	MET	A	178	28.135	11.774	-11.868	1.00	41.82	16
	ATOM	1394	CE	MET	A	178	28.027	13.573	-11.994	1.00	44.07	6
10	ATOM	1395	N	ARG	A	179	29.559	12.130	-17.573	1.00	19.57	7
	ATOM	1396	CA	ARG	A	179	29.384	12.934	-18.776	1.00	18.81	6
	ATOM	1397	C	ARG	A	179	27.950	12.914	-19.257	1.00	19.43	6
	ATOM	1398	O	ARG	A	179	27.182	12.014	-18.938	1.00	19.78	8
	ATOM	1399	CB	ARG	A	179	30.252	12.380	-19.936	1.00	20.44	6
15	ATOM	1400	CG	ARG	A	179	31.757	12.403	-19.680	1.00	21.94	6
	ATOM	1401	CD	ARG	A	179	32.547	11.665	-20.791	1.00	22.96	6
	ATOM	1402	NE	ARG	A	179	33.928	11.849	-20.377	1.00	24.17	7
	ATOM	1403	CZ	ARG	A	179	34.636	12.995	-20.379	1.00	23.08	6
	ATOM	1404	NH1	ARG	A	179	34.146	14.147	-20.883	1.00	22.58	7
20	ATOM	1405	NH2	ARG	A	179	35.872	12.925	-19.895	1.00	25.87	7
	ATOM	1406	N	ALA	A	180	27.526	13.954	-19.931	1.00	19.29	7
	ATOM	1407	CA	ALA	A	180	26.247	14.023	-20.609	1.00	20.57	6
	ATOM	1408	C	ALA	A	180	26.269	13.017	-21.785	1.00	20.46	6
	ATOM	1409	O	ALA	A	180	27.305	12.438	-22.089	1.00	20.53	8
25	ATOM	1410	CB	ALA	A	180	26.009	15.430	-21.100	1.00	20.95	6
	ATOM	1411	N	LYS	A	181	25.065	12.823	-22.355	1.00	23.00	7
	ATOM	1412	CA	LYS	A	181	24.978	11.807	-23.436	1.00	25.24	6
	ATOM	1413	C	LYS	A	181	25.745	12.150	-24.672	1.00	23.73	6
	ATOM	1414	O	LYS	A	181	26.108	11.238	-25.439	1.00	25.08	8
	ATOM	1415	CB	LYS	A	181	23.496	11.637	-23.802	1.00	25.36	6
30	ATOM	1416	CG	LYS	A	181	22.670	10.939	-22.755	1.00	29.60	6
	ATOM	1417	CD	LYS	A	181	23.217	9.642	-22.291	1.00	31.75	6
	ATOM	1418	N	ASP	A	182	26.027	13.427	-24.854	1.00	22.41	7
	ATOM	1419	CA	ASP	A	182	26.844	13.896	-25.958	1.00	23.30	6
35	ATOM	1420	C	ASP	A	182	28.319	13.944	-25.618	1.00	24.01	6
	ATOM	1421	O	ASP	A	182	29.102	14.328	-26.481	1.00	23.06	8
	ATOM	1422	CB	ASP	A	182	26.269	15.241	-26.435	1.00	23.96	6
	ATOM	1423	CG	ASP	A	182	26.307	16.365	-25.427	1.00	25.62	6
	ATOM	1424	OD1	ASP	A	182	26.954	16.241	-24.359	1.00	24.83	8
40	ATOM	1425	OD2	ASP	A	182	25.690	17.397	-25.755	1.00	27.42	8
	ATOM	1426	N	GLY	A	183	28.808	13.557	-24.413	1.00	19.95	7
	ATOM	1427	CA	GLY	A	183	30.201	13.464	-24.071	1.00	23.13	6
	ATOM	1428	C	GLY	A	183	30.666	14.607	-23.127	1.00	19.95	6
	ATOM	1429	O	GLY	A	183	31.799	14.532	-22.661	1.00	21.39	8
45	ATOM	1430	N	LEU	A	184	29.882	15.681	-23.119	1.00	19.14	7
	ATOM	1431	CA	LEU	A	184	30.339	16.847	-22.301	1.00	18.16	6
	ATOM	1432	C	LEU	A	184	30.494	16.470	-20.832	1.00	18.40	6
	ATOM	1433	O	LEU	A	184	29.587	15.913	-20.225	1.00	19.97	8
	ATOM	1434	CB	LEU	A	184	29.377	18.028	-22.486	1.00	18.63	6
50	ATOM	1435	CG	LEU	A	184	29.738	19.280	-21.652	1.00	17.34	6
	ATOM	1436	CD1	LEU	A	184	31.065	19.909	-22.111	1.00	19.12	6
	ATOM	1437	CD2	LEU	A	184	28.615	20.311	-21.740	1.00	19.88	6
	ATOM	1438	N	ALA	A	185	31.607	16.870	-20.184	1.00	16.12	7
	ATOM	1439	CA	ALA	A	185	31.782	16.555	-18.761	1.00	18.63	6
55	ATOM	1440	C	ALA	A	185	30.744	17.337	-17.942	1.00	17.79	6
	ATOM	1441	O	ALA	A	185	30.537	18.511	-18.196	1.00	18.57	8
	ATOM	1442	CB	ALA	A	185	33.237	16.872	-18.396	1.00	20.34	6
	ATOM	1443	N	LEU	A	186	30.024	16.634	-17.065	1.00	16.87	7
	ATOM	1444	CA	LEU	A	186	29.020	17.352	-16.271	1.00	16.99	6
60	ATOM	1445	C	LEU	A	186	29.790	18.284	-15.327	1.00	17.67	6
	ATOM	1446	O	LEU	A	186	30.768	17.866	-14.658	1.00	20.34	8
	ATOM	1447	CB	LEU	A	186	28.117	16.384	-15.513	1.00	16.87	6
	ATOM	1448	CG	LEU	A	186	27.300	15.408	-16.358	1.00	18.67	6
	ATOM	1449	CD1	LEU	A	186	26.353	14.626	-15.456	1.00	20.67	6
65	ATOM	1450	CD2	LEU	A	186	26.520	16.166	-17.415	1.00	17.31	6
	ATOM	1451	N	SER	A	187	29.252	19.481	-15.220	1.00	18.83	7
	ATOM	1452	CA	SER	A	187	29.915	20.486	-14.382	1.00	17.18	6
	ATOM	1453	C	SER	A	187	29.000	21.631	-14.105	1.00	17.64	6
	ATOM	1454	O	SER	A	187	28.216	22.057	-14.964	1.00	18.63	8
70	ATOM	1455	CB	SER	A	187	31.153	21.021	-15.151	1.00	20.23	6
	ATOM	1456	OG	SER	A	187	31.730	22.134	-14.430	1.00	20.91	8
	ATOM	1457	N	SER	A	188	29.176	22.275	-12.905	1.00	17.55	7
	ATOM	1458	CA	SER	A	188	28.463	23.548	-12.722	1.00	17.70	6
	ATOM	1459	C	SER	A	188	28.806	24.605	-13.755	1.00	17.74	6
	ATOM	1460	O	SER	A	188	28.014	25.522	-14.095	1.00	18.92	8

-56-

	ATOM	1461	CB	SER	A	188	28.799	24.124	-11.327	1.00	19.73	6
	ATOM	1462	OG	SER	A	188	30.220	24.296	-11.200	1.00	20.84	8
	ATOM	1463	N	ARG	A	189	29.969	24.554	-14.393	1.00	18.16	7
5	ATOM	1464	CA	ARG	A	189	30.424	25.497	-15.393	1.00	19.85	6
	ATOM	1465	C	ARG	A	189	29.538	25.498	-16.634	1.00	20.33	6
	ATOM	1466	O	ARG	A	189	29.484	26.473	-17.348	1.00	21.91	8
	ATOM	1467	CB	ARG	A	189	31.879	25.201	-15.823	1.00	20.55	6
	ATOM	1468	CG	ARG	A	189	32.801	25.314	-14.605	1.00	22.89	6
10	ATOM	1469	CD	ARG	A	189	34.254	25.061	-15.042	1.00	23.21	6
	ATOM	1470	NE	ARG	A	189	35.037	25.170	-13.785	1.00	25.97	7
	ATOM	1471	CZ	ARG	A	189	36.121	25.924	-13.683	1.00	28.29	6
	ATOM	1472	NH1	ARG	A	189	36.608	26.564	-14.711	1.00	26.60	7
	ATOM	1473	NH2	ARG	A	189	36.744	25.966	-12.487	1.00	28.41	7
15	ATOM	1474	N	ASN	A	190	28.914	24.324	-16.956	1.00	19.42	7
	ATOM	1475	CA	ASN	A	190	28.105	24.261	-18.156	1.00	19.64	6
	ATOM	1476	C	ASN	A	190	26.963	25.235	-18.114	1.00	22.61	6
	ATOM	1477	O	ASN	A	190	26.271	25.606	-19.109	1.00	23.27	8
	ATOM	1478	CB	ASN	A	190	27.544	22.841	-18.332	1.00	19.54	6
20	ATOM	1479	CG	ASN	A	190	28.675	21.842	-18.530	1.00	21.41	6
	ATOM	1480	OD1	ASN	A	190	28.471	20.621	-18.265	1.00	21.40	8
	ATOM	1481	ND2	ASN	A	190	29.819	22.309	-18.997	1.00	19.16	7
	ATOM	1497	N	GLY	A	191	26.554	25.616	-16.760	1.00	27.44	7
	ATOM	1498	CA	GLY	A	191	25.459	26.574	-16.600	1.00	28.04	6
25	ATOM	1499	C	GLY	A	191	25.750	27.966	-17.117	1.00	29.70	6
	ATOM	1500	O	GLY	A	191	24.790	28.715	-17.294	1.00	31.47	8
	ATOM	1482	N	TYR	A	192	26.966	28.311	-17.457	1.00	26.92	7
	ATOM	1483	CA	TYR	A	192	27.272	29.642	-17.970	1.00	29.88	6
	ATOM	1484	C	TYR	A	192	27.308	29.633	-19.479	1.00	29.91	6
30	ATOM	1485	O	TYR	A	192	27.538	30.724	-20.046	1.00	34.28	8
	ATOM	1486	CB	TYR	A	192	28.611	30.173	-17.427	1.00	30.32	6
	ATOM	1487	CG	TYR	A	192	28.459	30.366	-15.928	1.00	32.17	6
	ATOM	1488	CD1	TYR	A	192	28.608	29.256	-15.102	1.00	32.38	6
	ATOM	1489	CD2	TYR	A	192	28.097	31.585	-15.362	1.00	34.00	6
35	ATOM	1490	CE1	TYR	A	192	28.438	29.352	-13.751	1.00	35.21	6
	ATOM	1491	CE2	TYR	A	192	27.927	31.687	-13.985	1.00	34.55	6
	ATOM	1492	CZ	TYR	A	192	28.106	30.589	-13.195	1.00	36.66	6
	ATOM	1493	OH	TYR	A	192	27.942	30.636	-11.819	1.00	38.33	8
	ATOM	1494	N	LEU	A	193	27.090	28.487	-20.135	1.00	28.20	7
40	ATOM	1495	CA	LEU	A	193	27.054	28.479	-21.575	1.00	26.63	6
	ATOM	1496	C	LEU	A	193	25.718	28.903	-22.154	1.00	27.15	6
	ATOM	1497	O	LEU	A	193	24.697	28.434	-21.647	1.00	28.28	8
	ATOM	1498	CB	LEU	A	193	27.315	27.057	-22.112	1.00	26.20	6
	ATOM	1499	CG	LEU	A	193	28.613	26.402	-21.654	1.00	25.58	6
45	ATOM	1500	CD1	LEU	A	193	28.593	24.905	-21.877	1.00	24.08	6
	ATOM	1501	CD2	LEU	A	193	29.827	27.005	-22.390	1.00	27.77	6
	ATOM	1502	N	THR	A	194	25.679	29.616	-23.303	1.00	28.42	7
	ATOM	1503	CA	THR	A	194	24.376	29.825	-23.934	1.00	27.62	6
	ATOM	1504	C	THR	A	194	23.892	28.531	-24.561	1.00	25.74	6
50	ATOM	1505	O	THR	A	194	24.735	27.621	-24.723	1.00	26.48	8
	ATOM	1506	CB	THR	A	194	24.463	30.922	-25.011	1.00	29.34	6
	ATOM	1507	OG1	THR	A	194	25.465	30.535	-25.956	1.00	30.55	8
	ATOM	1508	CG2	THR	A	194	24.862	32.238	-24.353	1.00	32.65	6
	ATOM	1509	N	ALA	A	195	22.663	28.446	-25.043	1.00	25.15	7
55	ATOM	1510	CA	ALA	A	195	22.211	27.253	-25.755	1.00	25.73	6
	ATOM	1511	C	ALA	A	195	23.105	26.994	-26.972	1.00	28.33	6
	ATOM	1512	O	ALA	A	195	23.460	25.834	-27.241	1.00	28.09	8
	ATOM	1513	CB	ALA	A	195	20.768	27.315	-26.209	1.00	25.63	6
	ATOM	1514	N	GLU	A	196	23.486	28.068	-27.703	1.00	27.21	7
60	ATOM	1515	CA	GLU	A	196	24.366	27.886	-28.843	1.00	28.84	6
	ATOM	1516	C	GLU	A	196	25.718	27.351	-28.424	1.00	25.77	6
	ATOM	1517	O	GLU	A	196	26.282	26.445	-29.054	1.00	30.10	8
	ATOM	1518	CB	GLU	A	196	24.534	29.239	-29.570	1.00	31.35	6
	ATOM	1519	N	GLN	A	197	26.278	27.889	-27.328	1.00	26.45	7
65	ATOM	1520	CA	GLN	A	197	27.567	27.412	-26.855	1.00	25.85	6
	ATOM	1521	C	GLN	A	197	27.489	25.961	-26.330	1.00	25.97	6
	ATOM	1522	O	GLN	A	197	28.406	25.210	-26.618	1.00	25.79	8
	ATOM	1523	CB	GLN	A	197	28.157	28.273	-25.717	1.00	27.14	6
	ATOM	1524	CG	GLN	A	197	28.452	29.662	-26.408	1.00	29.94	6
70	ATOM	1525	CD	GLN	A	197	28.544	30.739	-25.358	1.00	31.03	6
	ATOM	1526	OE1	GLN	A	197	28.249	30.597	-24.174	1.00	31.48	8
	ATOM	1527	NE2	GLN	A	197	28.949	31.963	-25.739	1.00	30.58	7
	ATOM	1528	N	ARG	A	198	26.335	25.639	-25.736	1.00	23.62	7
	ATOM	1529	CA	ARG	A	198	26.151	24.282	-25.209	1.00	23.58	6
	ATOM	1530	C	ARG	A	198	26.204	23.282	-26.345	1.00	24.98	6

-57-

	ATOM	1531	O	ARG	A	198	26.761	22.214	-26.214	1.00	25.17	8
	ATOM	1532	CB	ARG	A	198	24.831	24.133	-24.454	1.00	22.16	6
	ATOM	1533	CG	ARG	A	198	24.576	22.689	-23.946	1.00	21.81	6
	ATOM	1534	CD	ARG	A	198	25.656	22.194	-23.010	1.00	22.56	6
5	ATOM	1535	NE	ARG	A	198	25.386	20.830	-22.532	1.00	21.88	7
	ATOM	1536	CZ	ARG	A	198	25.614	19.724	-23.247	1.00	24.32	6
	ATOM	1537	NH1	ARG	A	198	25.384	18.481	-22.824	1.00	23.45	7
	ATOM	1538	NH2	ARG	A	198	26.118	19.830	-24.477	1.00	25.14	7
10	ATOM	1539	N	LYS	A	199	25.707	23.649	-27.549	1.00	23.80	7
	ATOM	1540	CA	LYS	A	199	25.820	22.710	-28.684	1.00	22.66	6
	ATOM	1541	C	LYS	A	199	27.221	22.558	-29.202	1.00	22.59	6
	ATOM	1542	O	LYS	A	199	27.608	21.508	-29.753	1.00	24.00	8
	ATOM	1543	CB	LYS	A	199	24.855	23.272	-29.743	1.00	25.23	6
	ATOM	1544	CG	LYS	A	199	24.661	22.284	-30.903	1.00	27.40	6
15	ATOM	1545	CD	LYS	A	199	23.602	22.991	-31.802	1.00	32.35	6
	ATOM	1546	CE	LYS	A	199	23.336	22.059	-32.983	1.00	36.02	6
	ATOM	1547	NZ	LYS	A	199	22.311	22.674	-33.894	1.00	38.59	7
	ATOM	1548	N	ILE	A	200	28.111	23.556	-29.074	1.00	22.04	7
20	ATOM	1549	CA	ILE	A	200	29.513	23.458	-29.440	1.00	25.05	6
	ATOM	1550	C	ILE	A	200	30.415	22.725	-28.438	1.00	23.70	6
	ATOM	1551	O	ILE	A	200	31.347	21.980	-28.775	1.00	22.15	8
	ATOM	1552	CB	ILE	A	200	30.128	24.863	-29.575	1.00	25.43	6
	ATOM	1553	CG1	ILE	A	200	29.457	25.528	-30.809	1.00	26.99	6
25	ATOM	1554	CG2	ILE	A	200	31.644	24.911	-29.704	1.00	26.61	6
	ATOM	1555	CD1	ILE	A	200	29.746	27.029	-30.827	1.00	28.65	6
	ATOM	1556	N	ALA	A	201	29.987	22.836	-27.170	1.00	22.88	7
	ATOM	1557	CA	ALA	A	201	30.773	22.278	-26.053	1.00	24.80	6
	ATOM	1558	C	ALA	A	201	31.217	20.829	-26.110	1.00	23.52	6
30	ATOM	1559	O	ALA	A	201	32.363	20.607	-25.709	1.00	21.96	8
	ATOM	1560	CB	ALA	A	201	29.913	22.499	-24.781	1.00	24.70	6
	ATOM	1561	N	PRO	A	202	30.498	19.846	-26.659	1.00	24.18	7
	ATOM	1562	CA	PRO	A	202	30.946	18.473	-26.796	1.00	24.19	6
	ATOM	1563	C	PRO	A	202	32.191	18.288	-27.649	1.00	26.04	6
35	ATOM	1564	O	PRO	A	202	32.900	17.282	-27.556	1.00	25.77	8
	ATOM	1565	CB	PRO	A	202	29.759	17.693	-27.382	1.00	24.31	6
	ATOM	1566	CG	PRO	A	202	28.579	18.572	-27.068	1.00	23.02	6
	ATOM	1567	CD	PRO	A	202	29.073	19.991	-27.051	1.00	22.33	6
	ATOM	1568	N	GLY	A	203	32.559	19.351	-28.406	1.00	25.61	7
40	ATOM	1569	CA	GLY	A	203	33.779	19.327	-29.179	1.00	26.22	6
	ATOM	1570	C	GLY	A	203	35.012	19.196	-28.324	1.00	24.81	6
	ATOM	1571	O	GLY	A	203	36.061	18.750	-28.817	1.00	24.88	8
	ATOM	1572	N	LEU	A	204	34.999	19.724	-27.082	1.00	23.90	7
	ATOM	1573	CA	LEU	A	204	36.199	19.561	-26.254	1.00	23.72	6
45	ATOM	1574	C	LEU	A	204	36.550	18.119	-26.035	1.00	23.32	6
	ATOM	1575	O	LEU	A	204	37.689	17.689	-26.239	1.00	24.33	8
	ATOM	1576	CB	LEU	A	204	35.957	20.361	-24.936	1.00	24.53	6
	ATOM	1577	CG	LEU	A	204	37.111	20.290	-23.972	1.00	25.84	6
	ATOM	1578	CD1	LEU	A	204	38.425	20.791	-24.586	1.00	26.75	6
50	ATOM	1579	CD2	LEU	A	204	36.806	21.156	-22.742	1.00	26.68	6
	ATOM	1580	N	TYR	A	205	35.580	17.243	-25.663	1.00	21.57	7
	ATOM	1581	CA	TYR	A	205	35.804	15.836	-25.435	1.00	22.36	6
	ATOM	1582	C	TYR	A	205	36.200	15.116	-26.748	1.00	21.69	6
	ATOM	1583	O	TYR	A	205	37.041	14.212	-26.762	1.00	23.95	8
55	ATOM	1584	CB	TYR	A	205	34.533	15.211	-24.809	1.00	21.96	6
	ATOM	1585	CG	TYR	A	205	34.766	13.758	-24.505	1.00	25.55	6
	ATOM	1586	CD1	TYR	A	205	35.727	13.322	-23.619	1.00	27.86	6
	ATOM	1587	CD2	TYR	A	205	34.059	12.802	-25.253	1.00	29.16	6
	ATOM	1588	CE1	TYR	A	205	35.901	11.979	-23.364	1.00	30.07	6
60	ATOM	1589	CE2	TYR	A	205	34.261	11.448	-25.003	1.00	30.89	6
	ATOM	1590	CZ	TYR	A	205	35.158	11.053	-24.064	1.00	32.67	6
	ATOM	1591	OH	TYR	A	205	35.373	9.702	-23.839	1.00	36.20	8
	ATOM	1592	N	LYS	A	206	35.652	15.679	-27.833	1.00	23.35	7
	ATOM	1593	CA	LYS	A	206	36.040	15.114	-29.149	1.00	24.75	6
65	ATOM	1594	C	LYS	A	206	37.530	15.306	-29.401	1.00	24.74	6
	ATOM	1595	O	LYS	A	206	38.252	14.359	-29.757	1.00	26.16	8
	ATOM	1596	CB	LYS	A	206	35.223	15.740	-30.293	1.00	25.21	6
	ATOM	1597	CG	LYS	A	206	33.784	15.236	-30.295	1.00	30.61	6
	ATOM	1598	CD	LYS	A	206	33.118	15.648	-31.621	1.00	34.58	6
70	ATOM	1599	CE	LYS	A	206	31.600	15.547	-31.489	1.00	37.70	6
	ATOM	1600	NZ	LYS	A	206	30.951	15.934	-32.794	1.00	40.74	7
	ATOM	1601	N	VAL	A	207	37.995	16.518	-29.128	1.00	25.56	7
	ATOM	1602	CA	VAL	A	207	39.432	16.818	-29.324	1.00	26.41	6
	ATOM	1603	C	VAL	A	207	40.240	16.016	-28.333	1.00	26.75	6
	ATOM	1604	O	VAL	A	207	41.246	15.351	-28.662	1.00	26.06	8

-58-

	ATOM	1605	CB	VAL	A	207	39.714	18.318	-29.266	1.00	26.88	6
	ATOM	1606	CG1	VAL	A	207	41.212	18.590	-29.172	1.00	27.69	6
	ATOM	1607	CG2	VAL	A	207	39.062	18.967	-30.489	1.00	27.15	6
5	ATOM	1608	N	LEU	A	208	39.793	15.917	-27.065	1.00	26.81	7
	ATOM	1609	CA	LEU	A	208	40.472	15.110	-26.079	1.00	26.80	6
	ATOM	1610	C	LEU	A	208	40.555	13.645	-26.462	1.00	27.53	6
	ATOM	1611	O	LEU	A	208	41.616	13.017	-26.276	1.00	27.79	8
	ATOM	1612	CB	LEU	A	208	39.736	15.325	-24.732	1.00	28.31	6
10	ATOM	1613	CG	LEU	A	208	40.248	14.531	-23.535	1.00	31.14	6
	ATOM	1614	CD1	LEU	A	208	41.649	14.906	-23.142	1.00	31.37	6
	ATOM	1615	CD2	LEU	A	208	39.288	14.741	-22.347	1.00	33.29	6
	ATOM	1616	N	SER	A	209	39.539	13.042	-27.028	1.00	26.96	7
	ATOM	1617	CA	SER	A	209	39.536	11.655	-27.442	1.00	28.65	6
15	ATOM	1618	C	SER	A	209	40.427	11.463	-28.696	1.00	30.30	6
	ATOM	1619	O	SER	A	209	41.021	10.401	-28.829	1.00	29.86	8
	ATOM	1620	CB	SER	A	209	38.141	11.126	-27.751	1.00	32.08	6
	ATOM	1621	OG	SER	A	209	37.320	11.455	-26.630	1.00	36.96	8
	ATOM	1622	N	SER	A	210	40.502	12.521	-29.507	1.00	31.09	7
20	ATOM	1623	CA	SER	A	210	41.372	12.426	-30.703	1.00	33.89	6
	ATOM	1624	C	SER	A	210	42.826	12.447	-30.297	1.00	33.77	6
	ATOM	1625	O	SER	A	210	43.687	11.734	-30.842	1.00	34.87	8
	ATOM	1626	CB	SER	A	210	41.024	13.563	-31.655	1.00	36.51	6
	ATOM	1627	OG	SER	A	210	42.171	13.743	-32.490	1.00	42.40	8
25	ATOM	1628	N	ILE	A	211	43.172	13.190	-29.230	1.00	31.25	7
	ATOM	1629	CA	ILE	A	211	44.530	13.129	-28.705	1.00	30.79	6
	ATOM	1630	C	ILE	A	211	44.815	11.731	-28.188	1.00	31.65	6
	ATOM	1631	O	ILE	A	211	45.878	11.124	-28.405	1.00	31.20	8
	ATOM	1632	CB	ILE	A	211	44.710	14.154	-27.580	1.00	30.45	6
30	ATOM	1633	CG1	ILE	A	211	44.646	15.580	-28.137	1.00	29.16	6
	ATOM	1634	CG2	ILE	A	211	46.009	13.912	-26.797	1.00	28.20	6
	ATOM	1635	CD1	ILE	A	211	44.501	16.613	-27.014	1.00	28.78	6
	ATOM	1636	N	ALA	A	212	43.882	11.162	-27.426	1.00	31.19	7
	ATOM	1637	CA	ALA	A	212	44.069	9.828	-26.852	1.00	31.19	6
35	ATOM	1638	C	ALA	A	212	44.251	8.789	-27.955	1.00	33.70	6
	ATOM	1639	O	ALA	A	212	45.100	7.892	-27.832	1.00	34.72	8
	ATOM	1640	CB	ALA	A	212	42.879	9.427	-25.995	1.00	31.27	6
	ATOM	1641	N	ASP	A	213	43.478	8.916	-29.045	1.00	32.83	7
	ATOM	1642	CA	ASP	A	213	43.576	7.982	-30.167	1.00	34.55	6
40	ATOM	1643	C	ASP	A	213	45.008	7.998	-30.723	1.00	34.80	6
	ATOM	1644	O	ASP	A	213	45.616	6.938	-30.847	1.00	36.87	8
	ATOM	1645	CB	ASP	A	213	42.567	8.322	-31.256	1.00	33.87	6
	ATOM	1646	CG	ASP	A	213	41.145	7.900	-30.886	1.00	36.07	6
	ATOM	1647	OD1	ASP	A	213	40.932	7.091	-29.951	1.00	36.03	8
45	ATOM	1648	OD2	ASP	A	213	40.224	8.400	-31.585	1.00	36.99	8
	ATOM	1649	N	LYS	A	214	45.527	9.193	-30.994	1.00	34.39	7
	ATOM	1650	CA	LYS	A	214	46.892	9.357	-31.506	1.00	35.31	6
	ATOM	1651	C	LYS	A	214	47.904	8.782	-30.536	1.00	37.91	6
	ATOM	1652	O	LYS	A	214	48.900	8.106	-30.920	1.00	39.73	8
50	ATOM	1653	CB	LYS	A	214	47.196	10.833	-31.789	1.00	33.06	6
	ATOM	1654	CG	LYS	A	214	46.295	11.525	-32.774	1.00	33.68	6
	ATOM	1655	CD	LYS	A	214	46.733	12.968	-33.079	1.00	32.27	6
	ATOM	1656	CE	LYS	A	214	45.891	13.544	-34.215	1.00	33.88	6
	ATOM	1657	NZ	LYS	A	214	46.243	14.978	-34.497	1.00	35.57	7
55	ATOM	1658	N	LEU	A	215	47.726	9.056	-29.227	1.00	38.37	7
	ATOM	1659	CA	LEU	A	215	48.742	8.507	-28.299	1.00	41.26	6
	ATOM	1660	C	LEU	A	215	48.676	6.988	-28.267	1.00	42.76	6
	ATOM	1661	O	LEU	A	215	49.717	6.311	-28.250	1.00	43.43	8
	ATOM	1662	CB	LEU	A	215	48.615	9.016	-26.871	1.00	38.15	6
60	ATOM	1663	CG	LEU	A	215	48.941	10.483	-26.658	1.00	39.14	6
	ATOM	1664	CD1	LEU	A	215	48.406	10.973	-25.306	1.00	39.20	6
	ATOM	1665	CD2	LEU	A	215	50.441	10.749	-26.718	1.00	39.00	6
	ATOM	1666	N	GLN	A	216	47.493	6.407	-28.253	1.00	44.37	7
	ATOM	1667	CA	GLN	A	216	47.328	4.952	-28.225	1.00	47.10	6
65	ATOM	1668	C	GLN	A	216	47.833	4.272	-29.499	1.00	47.76	6
	ATOM	1669	O	GLN	A	216	48.153	3.081	-29.469	1.00	48.80	8
	ATOM	1670	CB	GLN	A	216	45.859	4.643	-27.991	1.00	48.55	6
	ATOM	1671	CG	GLN	A	216	45.452	3.303	-27.435	1.00	50.81	6
	ATOM	1672	CD	GLN	A	216	44.259	3.444	-26.493	1.00	53.17	6
70	ATOM	1673	OE1	GLN	A	216	43.252	4.063	-26.856	1.00	54.69	8
	ATOM	1674	NE2	GLN	A	216	44.354	2.898	-25.279	1.00	53.81	7
	ATOM	1675	N	ALA	A	217	47.944	4.977	-30.617	1.00	47.64	7
	ATOM	1676	CA	ALA	A	217	48.431	4.433	-31.869	1.00	48.49	6
	ATOM	1677	C	ALA	A	217	49.948	4.569	-31.997	1.00	48.68	6
	ATOM	1678	O	ALA	A	217	50.517	4.182	-33.024	1.00	51.00	8

-59-

	ATOM	1679	CB	ALA	A	217	47.789	5.138	-33.060	1.00	47.71	6
	ATOM	1680	N	GLY	A	218	50.612	5.211	-31.056	1.00	47.70	7
	ATOM	1681	CA	GLY	A	218	52.037	5.390	-31.027	1.00	46.44	6
5	ATOM	1682	C	GLY	A	218	52.539	6.780	-31.316	1.00	47.59	6
	ATOM	1683	O	GLY	A	218	53.771	6.979	-31.285	1.00	47.50	8
	ATOM	1684	N	GLU	A	219	51.677	7.755	-31.607	1.00	45.89	7
	ATOM	1685	CA	GLU	A	219	52.216	9.086	-31.891	1.00	46.96	6
	ATOM	1686	C	GLU	A	219	52.912	9.624	-30.651	1.00	48.26	6
10	ATOM	1687	O	GLU	A	219	52.403	9.484	-29.530	1.00	48.86	8
	ATOM	1688	CB	GLU	A	219	51.146	10.071	-32.380	1.00	47.88	6
	ATOM	1689	CG	GLU	A	219	50.460	9.695	-33.672	1.00	48.05	6
	ATOM	1690	CD	GLU	A	219	49.744	10.817	-34.384	1.00	50.68	6
	ATOM	1691	OE1	GLU	A	219	50.134	12.015	-34.408	1.00	51.01	8
	ATOM	1692	OE2	GLU	A	219	48.702	10.497	-35.025	1.00	52.09	8
15	ATOM	1693	N	ARG	A	220	54.135	10.154	-30.831	1.00	47.68	7
	ATOM	1694	CA	ARG	A	220	54.868	10.698	-29.694	1.00	47.37	6
	ATOM	1695	C	ARG	A	220	55.402	12.091	-29.989	1.00	47.62	6
	ATOM	1696	O	ARG	A	220	56.106	12.622	-29.125	1.00	49.49	8
20	ATOM	1697	CB	ARG	A	220	56.014	9.790	-29.239	1.00	46.78	6
	ATOM	1698	CG	ARG	A	220	55.570	8.463	-28.643	1.00	46.54	6
	ATOM	1699	CD	ARG	A	220	54.878	8.628	-27.293	1.00	45.80	6
	ATOM	1700	NE	ARG	A	220	54.371	7.359	-26.801	1.00	45.04	7
	ATOM	1701	CZ	ARG	A	220	53.281	6.683	-27.074	1.00	44.93	6
25	ATOM	1702	NH1	ARG	A	220	52.341	7.093	-27.930	1.00	45.42	7
	ATOM	1703	NH2	ARG	A	220	53.080	5.516	-26.476	1.00	44.28	7
	ATOM	1704	N	ASP	A	221	54.976	12.756	-31.052	1.00	48.60	7
	ATOM	1705	CA	ASP	A	221	55.381	14.161	-31.242	1.00	48.15	6
	ATOM	1706	C	ASP	A	221	54.296	15.005	-30.557	1.00	46.06	6
30	ATOM	1707	O	ASP	A	221	53.379	15.515	-31.197	1.00	44.76	8
	ATOM	1708	CB	ASP	A	221	55.576	14.527	-32.691	1.00	50.20	6
	ATOM	1709	CG	ASP	A	221	56.053	15.928	-32.988	1.00	53.21	6
	ATOM	1710	OD1	ASP	A	221	56.188	16.801	-32.101	1.00	53.81	8
	ATOM	1711	OD2	ASP	A	221	56.309	16.204	-34.191	1.00	55.09	8
35	ATOM	1712	N	LEU	A	222	54.465	15.167	-29.249	1.00	43.92	7
	ATOM	1713	CA	LEU	A	222	53.451	15.829	-28.427	1.00	42.81	6
	ATOM	1714	C	LEU	A	222	53.215	17.271	-28.774	1.00	43.64	6
	ATOM	1715	O	LEU	A	222	52.066	17.762	-28.789	1.00	41.82	8
	ATOM	1716	CB	LEU	A	222	53.894	15.652	-26.952	1.00	43.09	6
40	ATOM	1717	CG	LEU	A	222	54.196	14.191	-26.578	1.00	41.83	6
	ATOM	1718	CD1	LEU	A	222	54.442	14.033	-25.081	1.00	42.53	6
	ATOM	1719	CD2	LEU	A	222	53.086	13.237	-26.991	1.00	41.15	6
	ATOM	1720	N	ASP	A	223	54.285	18.012	-29.105	1.00	43.23	7
	ATOM	1721	CA	ASP	A	223	54.124	19.416	-29.472	1.00	44.33	6
45	ATOM	1722	C	ASP	A	223	53.223	19.562	-30.688	1.00	44.26	6
	ATOM	1723	O	ASP	A	223	52.401	20.490	-30.770	1.00	45.10	8
	ATOM	1724	CB	ASP	A	223	55.508	20.042	-29.717	1.00	45.77	6
	ATOM	1725	N	GLU	A	224	53.398	18.654	-31.651	1.00	44.43	7
	ATOM	1726	CA	GLU	A	224	52.583	18.676	-32.863	1.00	45.57	6
50	ATOM	1727	C	GLU	A	224	51.126	18.332	-32.533	1.00	41.13	6
	ATOM	1728	O	GLU	A	224	50.187	18.995	-32.967	1.00	40.57	8
	ATOM	1729	CB	GLU	A	224	53.146	17.723	-33.915	1.00	49.14	6
	ATOM	1730	CG	GLU	A	224	52.327	17.645	-35.186	1.00	53.71	6
	ATOM	1731	CD	GLU	A	224	52.241	18.926	-35.991	1.00	57.27	6
55	ATOM	1732	OE1	GLU	A	224	52.627	20.028	-35.530	1.00	58.34	8
	ATOM	1733	OE2	GLU	A	224	51.738	18.792	-37.141	1.00	59.44	8
	ATOM	1734	N	ILE	A	225	50.928	17.234	-31.837	1.00	38.07	7
	ATOM	1735	CA	ILE	A	225	49.602	16.821	-31.360	1.00	36.44	6
	ATOM	1736	C	ILE	A	225	48.838	17.929	-30.641	1.00	35.31	6
60	ATOM	1737	O	ILE	A	225	47.630	18.075	-30.873	1.00	34.79	8
	ATOM	1738	CB	ILE	A	225	49.745	15.630	-30.401	1.00	36.23	6
	ATOM	1739	CG1	ILE	A	225	50.310	14.449	-31.200	1.00	36.60	6
	ATOM	1740	CG2	ILE	A	225	48.432	15.233	-29.722	1.00	36.18	6
	ATOM	1741	CD1	ILE	A	225	50.515	13.174	-30.428	1.00	37.76	6
65	ATOM	1742	N	ILE	A	226	49.522	18.680	-29.780	1.00	33.53	7
	ATOM	1743	CA	ILE	A	226	48.922	19.759	-29.025	1.00	33.52	6
	ATOM	1744	C	ILE	A	226	48.614	20.969	-29.881	1.00	33.80	6
	ATOM	1745	O	ILE	A	226	47.581	21.655	-29.737	1.00	32.30	8
	ATOM	1746	CB	ILE	A	226	49.877	20.107	-27.843	1.00	34.98	6
70	ATOM	1747	CG1	ILE	A	226	49.847	18.937	-26.874	1.00	34.99	6
	ATOM	1748	CG2	ILE	A	226	49.490	21.417	-27.159	1.00	34.94	6
	ATOM	1749	CD1	ILE	A	226	50.657	19.117	-25.611	1.00	36.97	6
	ATOM	1750	N	THR	A	227	49.527	21.261	-30.830	1.00	33.69	7
	ATOM	1751	CA	THR	A	227	49.287	22.418	-31.697	1.00	34.02	6
	ATOM	1752	C	THR	A	227	48.040	22.160	-32.526	1.00	32.93	6

-60-

	ATOM	1753	O	THR	A	227	47.183	23.034	-32.604	1.00	33.21	8
	ATOM	1754	CB	THR	A	227	50.469	22.754	-32.630	1.00	36.23	6
	ATOM	1755	OG1	THR	A	227	51.656	22.905	-31.839	1.00	38.63	8
5	ATOM	1756	CG2	THR	A	227	50.229	24.059	-33.378	1.00	37.54	6
	ATOM	1757	N	ILE	A	228	47.887	20.967	-33.060	1.00	33.57	7
	ATOM	1758	CA	ILE	A	228	46.742	20.647	-33.899	1.00	33.85	6
	ATOM	1759	C	ILE	A	228	45.453	20.703	-33.074	1.00	33.32	6
	ATOM	1760	O	ILE	A	228	44.417	21.205	-33.482	1.00	31.47	8
10	ATOM	1761	CB	ILE	A	228	46.908	19.275	-34.533	1.00	36.08	6
	ATOM	1762	CG1	ILE	A	228	48.002	19.323	-35.634	1.00	39.34	6
	ATOM	1763	CG2	ILE	A	228	45.610	18.758	-35.136	1.00	35.68	6
	ATOM	1764	CD1	ILE	A	228	48.385	17.919	-36.092	1.00	39.59	6
	ATOM	1765	N	ALA	A	229	45.597	20.146	-31.859	1.00	33.09	7
15	ATOM	1766	CA	ALA	A	229	44.441	20.114	-30.930	1.00	31.53	6
	ATOM	1767	C	ALA	A	229	43.948	21.497	-30.607	1.00	28.89	6
	ATOM	1768	O	ALA	A	229	42.733	21.771	-30.644	1.00	28.46	8
	ATOM	1769	CB	ALA	A	229	44.898	19.315	-29.707	1.00	31.42	6
	ATOM	1770	N	GLY	A	230	44.836	22.471	-30.407	1.00	29.20	7
20	ATOM	1771	CA	GLY	A	230	44.485	23.857	-30.166	1.00	30.51	6
	ATOM	1772	C	GLY	A	230	43.797	24.472	-31.372	1.00	31.48	6
	ATOM	1773	O	GLY	A	230	42.759	25.155	-31.288	1.00	33.24	8
	ATOM	1774	N	GLN	A	231	44.374	24.217	-32.569	1.00	33.19	7
	ATOM	1775	CA	GLN	A	231	43.812	24.700	-33.823	1.00	33.48	6
25	ATOM	1776	C	GLN	A	231	42.396	24.206	-34.027	1.00	32.96	6
	ATOM	1777	O	GLN	A	231	41.476	24.995	-34.324	1.00	34.21	8
	ATOM	1778	CB	GLN	A	231	44.704	24.245	-35.003	1.00	34.34	6
	ATOM	1779	CG	GLN	A	231	46.007	25.041	-35.007	1.00	36.14	6
	ATOM	1780	CD	GLN	A	231	47.002	24.556	-36.052	1.00	38.53	6
30	ATOM	1781	OE1	GLN	A	231	46.812	23.541	-36.732	1.00	39.14	8
	ATOM	1782	NE2	GLN	A	231	48.085	25.312	-36.189	1.00	39.12	7
	ATOM	1783	N	GLU	A	232	42.214	22.900	-33.801	1.00	31.08	7
	ATOM	1784	CA	GLU	A	232	40.897	22.280	-33.907	1.00	33.90	6
	ATOM	1785	C	GLU	A	232	39.897	22.898	-32.923	1.00	32.79	6
35	ATOM	1786	O	GLU	A	232	38.785	23.235	-33.345	1.00	30.71	8
	ATOM	1787	CB	GLU	A	232	40.956	20.772	-33.659	1.00	36.16	6
	ATOM	1788	CG	GLU	A	232	41.681	19.963	-34.705	1.00	40.99	6
	ATOM	1789	CD	GLU	A	232	41.956	18.526	-34.336	1.00	43.88	6
	ATOM	1790	OE1	GLU	A	232	42.231	18.222	-33.162	1.00	46.75	8
40	ATOM	1791	OE2	GLU	A	232	41.978	17.624	-35.213	1.00	46.96	8
	ATOM	1792	N	LEU	A	233	40.279	23.075	-31.654	1.00	31.79	7
	ATOM	1793	CA	LEU	A	233	39.390	23.738	-30.717	1.00	31.75	6
	ATOM	1794	C	LEU	A	233	39.053	25.159	-31.151	1.00	30.93	6
	ATOM	1795	O	LEU	A	233	37.914	25.617	-31.117	1.00	29.58	8
45	ATOM	1796	CB	LEU	A	233	40.002	23.804	-29.306	1.00	28.67	6
	ATOM	1797	CG	LEU	A	233	40.122	22.439	-28.598	1.00	29.48	6
	ATOM	1798	CD1	LEU	A	233	41.084	22.505	-27.425	1.00	29.09	6
	ATOM	1799	CD2	LEU	A	233	38.712	21.976	-28.189	1.00	30.10	6
	ATOM	1800	N	ASN	A	234	40.083	25.889	-31.615	1.00	32.79	7
50	ATOM	1801	CA	ASN	A	234	39.861	27.288	-32.011	1.00	33.77	6
	ATOM	1802	C	ASN	A	234	38.946	27.388	-33.220	1.00	31.44	6
	ATOM	1803	O	ASN	A	234	38.071	28.254	-33.258	1.00	32.82	8
	ATOM	1804	CB	ASN	A	234	41.220	27.972	-32.243	1.00	36.16	6
	ATOM	1805	CG	ASN	A	234	41.890	28.295	-30.919	1.00	39.98	6
55	ATOM	1806	OD1	ASN	A	234	41.296	28.257	-29.838	1.00	40.76	8
	ATOM	1807	ND2	ASN	A	234	43.185	28.592	-30.922	1.00	39.55	7
	ATOM	1808	N	GLU	A	235	39.068	26.440	-34.127	1.00	31.44	7
	ATOM	1809	CA	GLU	A	235	38.223	26.392	-35.306	1.00	34.68	6
	ATOM	1810	C	GLU	A	235	36.779	26.082	-34.971	1.00	34.35	6
60	ATOM	1811	O	GLU	A	235	35.878	26.565	-35.629	1.00	35.56	8
	ATOM	1812	CB	GLU	A	235	38.763	25.314	-36.244	1.00	36.35	6
	ATOM	1813	N	LYS	A	236	36.532	25.307	-33.908	1.00	36.15	7
	ATOM	1814	CA	LYS	A	236	35.169	24.977	-33.488	1.00	35.47	6
	ATOM	1815	C	LYS	A	236	34.483	26.106	-32.738	1.00	34.87	6
65	ATOM	1816	O	LYS	A	236	33.253	26.085	-32.561	1.00	36.38	8
	ATOM	1817	CB	LYS	A	236	35.213	23.748	-32.577	1.00	37.47	6
	ATOM	1818	CG	LYS	A	236	35.609	22.450	-33.245	1.00	38.51	6
	ATOM	1819	CD	LYS	A	236	35.643	21.345	-32.192	1.00	40.94	6
	ATOM	1820	CE	LYS	A	236	36.184	20.083	-32.827	1.00	42.93	6
70	ATOM	1821	NZ	LYS	A	236	36.231	18.973	-31.850	1.00	45.15	7
	ATOM	1822	N	GLY	A	237	35.225	27.094	-32.274	1.00	33.61	7
	ATOM	1823	CA	GLY	A	237	34.660	28.241	-31.576	1.00	33.28	6
	ATOM	1824	C	GLY	A	237	35.127	28.401	-30.157	1.00	32.89	6
	ATOM	1825	O	GLY	A	237	34.644	29.291	-29.429	1.00	36.87	8
	ATOM	1826	N	PHE	A	238	36.017	27.546	-29.668	1.00	30.90	7

-61-

	ATOM	1827	CA	PHE	A	238	36.629	27.664	-28.380	1.00	31.61	6
	ATOM	1828	C	PHE	A	238	37.817	28.641	-28.417	1.00	35.03	6
	ATOM	1829	O	PHE	A	238	38.191	29.022	-29.528	1.00	37.95	8
5	ATOM	1830	CB	PHE	A	238	37.201	26.338	-27.875	1.00	29.76	6
	ATOM	1831	CG	PHE	A	238	36.165	25.258	-27.686	1.00	30.50	6
	ATOM	1832	CD1	PHE	A	238	35.712	24.500	-28.727	1.00	29.47	6
	ATOM	1833	CD2	PHE	A	238	35.679	24.979	-26.414	1.00	31.42	6
	ATOM	1834	CE1	PHE	A	238	34.752	23.501	-28.555	1.00	31.11	6
10	ATOM	1835	CE2	PHE	A	238	34.731	23.986	-26.233	1.00	29.77	6
	ATOM	1836	CZ	PHE	A	238	34.284	23.235	-27.279	1.00	29.29	6
	ATOM	1837	N	ARG	A	239	38.388	28.963	-27.268	1.00	34.76	7
	ATOM	1838	CA	ARG	A	239	39.674	29.645	-27.216	1.00	35.49	6
	ATOM	1839	C	ARG	A	239	40.472	28.742	-26.270	1.00	35.32	6
15	ATOM	1840	O	ARG	A	239	40.308	28.724	-25.057	1.00	32.89	8
	ATOM	1841	CB	ARG	A	239	39.721	31.088	-26.754	1.00	37.36	6
	ATOM	1842	CG	ARG	A	239	39.226	32.068	-27.822	1.00	39.64	6
	ATOM	1843	N	ALA	A	240	41.233	27.877	-26.931	1.00	36.31	7
	ATOM	1844	CA	ALA	A	240	42.124	26.921	-26.293	1.00	36.79	6
20	ATOM	1845	C	ALA	A	240	42.906	27.617	-25.203	1.00	38.54	6
	ATOM	1846	O	ALA	A	240	43.360	28.735	-25.495	1.00	39.25	8
	ATOM	1847	CB	ALA	A	240	43.087	26.347	-27.333	1.00	36.86	6
	ATOM	1848	N	ASP	A	241	43.035	27.053	-24.024	1.00	39.01	7
	ATOM	1849	CA	ASP	A	241	43.689	27.789	-22.947	1.00	42.42	6
25	ATOM	1850	C	ASP	A	241	44.867	27.010	-22.396	1.00	43.73	6
	ATOM	1851	O	ASP	A	241	45.894	27.608	-22.061	1.00	46.19	8
	ATOM	1852	CB	ASP	A	241	42.686	28.105	-21.828	1.00	43.72	6
	ATOM	1853	CG	ASP	A	241	43.319	28.991	-20.771	1.00	46.29	6
	ATOM	1854	OD1	ASP	A	241	43.712	30.124	-21.130	1.00	47.38	8
30	ATOM	1855	OD2	ASP	A	241	43.433	28.560	-19.610	1.00	46.21	8
	ATOM	1856	N	ASP	A	242	44.733	25.690	-22.292	1.00	41.53	7
	ATOM	1857	CA	ASP	A	242	45.828	24.876	-21.764	1.00	39.46	6
	ATOM	1858	C	ASP	A	242	45.607	23.442	-22.177	1.00	37.10	6
	ATOM	1859	O	ASP	A	242	44.496	22.895	-22.059	1.00	34.02	8
35	ATOM	1860	CB	ASP	A	242	45.908	25.001	-20.242	1.00	43.32	6
	ATOM	1861	CG	ASP	A	242	47.103	24.275	-19.661	1.00	47.37	6
	ATOM	1862	OD1	ASP	A	242	46.980	23.437	-18.736	1.00	49.59	8
	ATOM	1863	OD2	ASP	A	242	48.231	24.530	-20.158	1.00	50.50	8
	ATOM	1864	N	ILE	A	243	46.597	22.785	-22.750	1.00	33.48	7
40	ATOM	1865	CA	ILE	A	243	46.550	21.419	-23.193	1.00	32.08	6
	ATOM	1866	C	ILE	A	243	47.853	20.812	-22.718	1.00	33.41	6
	ATOM	1867	O	ILE	A	243	48.895	21.390	-23.062	1.00	32.28	8
	ATOM	1868	CB	ILE	A	243	46.424	21.205	-24.719	1.00	33.19	6
	ATOM	1869	CG1	ILE	A	243	45.141	21.847	-25.222	1.00	33.31	6
45	ATOM	1870	CG2	ILE	A	243	46.504	19.703	-24.995	1.00	32.88	6
	ATOM	1871	CD1	ILE	A	243	44.892	21.792	-26.713	1.00	33.52	6
	ATOM	1872	N	GLN	A	244	47.829	19.735	-21.975	1.00	33.31	7
	ATOM	1873	CA	GLN	A	244	49.003	19.097	-21.436	1.00	35.24	6
	ATOM	1874	C	GLN	A	244	48.849	17.592	-21.483	1.00	34.74	6
50	ATOM	1875	O	GLN	A	244	47.741	17.056	-21.422	1.00	33.25	8
	ATOM	1876	CB	GLN	A	244	49.300	19.528	-19.967	1.00	39.02	6
	ATOM	1877	CG	GLN	A	244	49.773	20.962	-19.905	1.00	43.89	6
	ATOM	1878	CD	GLN	A	244	50.076	21.564	-18.569	1.00	47.28	6
	ATOM	1879	OE1	GLN	A	244	50.148	20.870	-17.548	1.00	48.52	8
55	ATOM	1880	NE2	GLN	A	244	50.259	22.895	-18.597	1.00	49.46	7
	ATOM	1881	N	ILE	A	245	49.943	16.870	-21.716	1.00	31.86	7
	ATOM	1882	CA	ILE	A	245	50.000	15.439	-21.801	1.00	31.75	6
	ATOM	1883	C	ILE	A	245	51.110	14.967	-20.852	1.00	33.59	6
	ATOM	1884	O	ILE	A	245	52.183	15.586	-20.888	1.00	36.14	8
60	ATOM	1885	CB	ILE	A	245	50.299	14.888	-23.213	1.00	33.28	6
	ATOM	1886	CG1	ILE	A	245	49.188	15.324	-24.177	1.00	32.78	6
	ATOM	1887	CG2	ILE	A	245	50.470	13.387	-23.164	1.00	33.13	6
	ATOM	1888	CD1	ILE	A	245	49.424	15.049	-25.648	1.00	33.13	6
	ATOM	1889	N	ARG	A	246	50.827	14.054	-19.946	1.00	34.84	7
65	ATOM	1890	CA	ARG	A	246	51.816	13.609	-18.982	1.00	35.92	6
	ATOM	1891	C	ARG	A	246	51.687	12.122	-18.690	1.00	35.36	6
	ATOM	1892	O	ARG	A	246	50.697	11.461	-18.911	1.00	35.88	8
	ATOM	1893	CB	ARG	A	246	51.713	14.251	-17.589	1.00	36.79	6
	ATOM	1894	CG	ARG	A	246	51.674	15.747	-17.458	1.00	41.24	6
70	ATOM	1895	CD	ARG	A	246	53.032	16.284	-17.914	1.00	46.18	6
	ATOM	1896	NE	ARG	A	246	53.251	17.654	-17.502	1.00	49.48	7
	ATOM	1897	CZ	ARG	A	246	53.913	18.040	-16.420	1.00	51.58	6
	ATOM	1898	NH1	ARG	A	246	54.466	17.155	-15.603	1.00	51.91	7
	ATOM	1899	NH2	ARG	A	246	54.006	19.352	-16.229	1.00	53.89	7
	ATOM	1900	N	ASP	A	247	52.730	11.616	-18.003	1.00	35.81	7

-62-

	ATOM	1901	CA	ASP	A	247	52.753	10.248	-17.537	1.00	34.88	6
	ATOM	1902	C	ASP	A	247	51.652	10.087	-16.495	1.00	31.75	6
	ATOM	1903	O	ASP	A	247	51.690	10.908	-15.584	1.00	32.95	8
5	ATOM	1904	CB	ASP	A	247	54.146	9.952	-16.954	1.00	37.68	6
	ATOM	1905	CG	ASP	A	247	54.195	8.479	-16.611	1.00	39.66	6
	ATOM	1906	OD1	ASP	A	247	53.482	8.015	-15.710	1.00	41.79	8
	ATOM	1907	OD2	ASP	A	247	54.924	7.748	-17.284	1.00	42.94	8
	ATOM	1908	N	ALA	A	248	50.712	9.185	-16.600	1.00	33.81	7
10	ATOM	1909	CA	ALA	A	248	49.616	9.156	-15.609	1.00	32.51	6
	ATOM	1910	C	ALA	A	248	50.041	8.675	-14.232	1.00	34.35	6
	ATOM	1911	O	ALA	A	248	49.399	9.063	-13.249	1.00	33.85	8
	ATOM	1912	CB	ALA	A	248	48.499	8.253	-16.070	1.00	33.01	6
	ATOM	1913	N	ASP	A	249	51.057	7.825	-14.103	1.00	36.10	7
15	ATOM	1914	CA	ASP	A	249	51.462	7.281	-12.822	1.00	35.70	6
	ATOM	1915	C	ASP	A	249	52.421	8.185	-12.073	1.00	33.40	6
	ATOM	1916	O	ASP	A	249	52.399	8.230	-10.818	1.00	31.30	8
	ATOM	1917	CB	ASP	A	249	52.152	5.916	-13.031	1.00	39.11	6
	ATOM	1918	CG	ASP	A	249	51.137	5.007	-13.715	1.00	43.20	6
20	ATOM	1919	OD1	ASP	A	249	50.028	4.826	-13.134	1.00	45.31	8
	ATOM	1920	OD2	ASP	A	249	51.423	4.514	-14.817	1.00	43.99	8
	ATOM	1921	N	THR	A	250	53.275	8.844	-12.857	1.00	31.16	7
	ATOM	1922	CA	THR	A	250	54.301	9.667	-12.240	1.00	32.87	6
	ATOM	1923	C	THR	A	250	54.087	11.144	-12.416	1.00	32.81	6
25	ATOM	1924	O	THR	A	250	54.760	11.935	-11.789	1.00	30.56	8
	ATOM	1925	CB	THR	A	250	55.740	9.378	-12.792	1.00	34.12	6
	ATOM	1926	OG1	THR	A	250	55.779	9.795	-14.158	1.00	34.42	8
	ATOM	1927	CG2	THR	A	250	56.080	7.911	-12.637	1.00	34.28	6
	ATOM	1928	N	LEU	A	251	53.281	11.587	-13.365	1.00	32.56	7
30	ATOM	1929	CA	LEU	A	251	52.972	12.978	-13.672	1.00	34.35	6
	ATOM	1930	C	LEU	A	251	54.124	13.689	-14.360	1.00	35.41	6
	ATOM	1931	O	LEU	A	251	54.093	14.893	-14.592	1.00	35.99	8
	ATOM	1932	CB	LEU	A	251	52.494	13.758	-12.418	1.00	33.68	6
	ATOM	1933	CG	LEU	A	251	51.220	13.147	-11.792	1.00	34.55	6
35	ATOM	1934	CD1	LEU	A	251	50.797	13.969	-10.573	1.00	35.91	6
	ATOM	1935	CD2	LEU	A	251	50.101	13.012	-12.821	1.00	35.43	6
	ATOM	1936	N	LEU	A	252	55.194	12.962	-14.695	1.00	39.58	7
	ATOM	1937	CA	LEU	A	252	56.323	13.507	-15.418	1.00	40.96	6
	ATOM	1938	C	LEU	A	252	55.945	13.614	-16.874	1.00	43.27	6
40	ATOM	1939	O	LEU	A	252	54.906	13.129	-17.318	1.00	40.97	8
	ATOM	1940	CB	LEU	A	252	57.550	12.584	-15.264	1.00	42.55	6
	ATOM	1941	CG	LEU	A	252	58.072	12.496	-13.823	1.00	43.46	6
	ATOM	1942	CD1	LEU	A	252	59.196	11.476	-13.685	1.00	44.26	6
	ATOM	1943	CD2	LEU	A	252	58.546	13.868	-13.341	1.00	43.34	6
45	ATOM	1944	N	GLU	A	253	56.855	14.189	-17.659	1.00	46.27	7
	ATOM	1945	CA	GLU	A	253	56.716	14.144	-19.109	1.00	48.94	6
	ATOM	1946	C	GLU	A	253	56.642	12.706	-19.612	1.00	48.01	6
	ATOM	1947	O	GLU	A	253	57.291	11.928	-18.871	1.00	48.08	8
	ATOM	1948	CB	GLU	A	253	57.877	14.878	-19.783	1.00	52.86	6
50	ATOM	1949	CG	GLU	A	253	57.914	16.371	-19.500	1.00	57.25	6
	ATOM	1950	CD	GLU	A	253	56.720	17.104	-20.077	1.00	60.45	6
	ATOM	1951	OE1	GLU	A	253	56.308	16.771	-21.207	1.00	61.73	8
	ATOM	1952	OE2	GLU	A	253	56.194	18.011	-19.397	1.00	61.77	8
	ATOM	1953	N	VAL	A	254	55.835	12.324	-20.596	1.00	48.66	7
55	ATOM	1954	CA	VAL	A	254	55.849	10.887	-20.872	1.00	49.85	6
	ATOM	1955	C	VAL	A	254	57.149	10.638	-21.614	1.00	51.30	6
	ATOM	1956	O	VAL	A	254	57.658	11.494	-22.340	1.00	49.27	8
	ATOM	1957	CB	VAL	A	254	54.576	10.399	-21.614	1.00	51.06	6
	ATOM	1958	CG1	VAL	A	254	53.600	11.541	-21.825	1.00	50.21	6
60	ATOM	1959	CG2	VAL	A	254	54.935	9.757	-22.940	1.00	51.39	6
	ATOM	1960	N	SER	A	255	57.636	9.432	-21.398	1.00	50.78	7
	ATOM	1961	CA	SER	A	255	58.878	8.951	-21.946	1.00	52.29	6
	ATOM	1962	C	SER	A	255	58.718	7.516	-22.423	1.00	53.07	6
	ATOM	1963	O	SER	A	255	57.625	6.965	-22.444	1.00	53.08	8
65	ATOM	1964	CB	SER	A	255	59.978	8.985	-20.878	1.00	51.99	6
	ATOM	1965	OG	SER	A	255	59.761	7.859	-20.013	1.00	51.83	8
	ATOM	1966	N	GLU	A	256	59.844	6.858	-22.692	1.00	55.01	7
	ATOM	1967	CA	GLU	A	256	59.903	5.485	-23.155	1.00	55.63	6
	ATOM	1968	C	GLU	A	256	59.251	4.493	-22.207	1.00	55.82	6
70	ATOM	1969	O	GLU	A	256	58.566	3.543	-22.591	1.00	55.91	8
	ATOM	1970	CB	GLU	A	256	61.380	5.091	-23.350	1.00	56.43	6
	ATOM	1971	N	THR	A	257	59.458	4.732	-20.919	1.00	55.14	7
	ATOM	1972	CA	THR	A	257	58.921	3.928	-19.846	1.00	54.05	6
	ATOM	1973	C	THR	A	257	57.443	4.151	-19.554	1.00	51.69	6
	ATOM	1974	O	THR	A	257	56.836	3.301	-18.887	1.00	51.58	8

-63-

	ATOM	1975	CB	THR	A	257	59.723	4.223	-18.554	1.00	55.07	6
	ATOM	1976	OG1	THR	A	257	59.404	5.533	-18.065	1.00	56.77	8
	ATOM	1977	CG2	THR	A	257	61.215	4.150	-18.828	1.00	55.65	6
5	ATOM	1978	N	SER	A	258	56.834	5.252	-20.000	1.00	49.85	7
	ATOM	1979	CA	SER	A	258	55.426	5.481	-19.663	1.00	46.23	6
	ATOM	1980	C	SER	A	258	54.484	4.382	-20.104	1.00	46.46	6
	ATOM	1981	O	SER	A	258	54.511	3.984	-21.269	1.00	47.83	8
	ATOM	1982	CB	SER	A	258	54.950	6.783	-20.306	1.00	44.06	6
10	ATOM	1983	OG	SER	A	258	55.742	7.841	-19.839	1.00	40.94	8
	ATOM	1984	N	LYS	A	259	53.626	3.905	-19.221	1.00	46.05	7
	ATOM	1985	CA	LYS	A	259	52.624	2.902	-19.512	1.00	46.69	6
	ATOM	1986	C	LYS	A	259	51.252	3.551	-19.739	1.00	45.85	6
	ATOM	1987	O	LYS	A	259	50.329	3.046	-20.369	1.00	45.29	8
15	ATOM	1988	CB	LYS	A	259	52.455	1.886	-18.382	1.00	46.44	6
	ATOM	1989	CG	LYS	A	259	53.726	1.200	-17.920	1.00	47.93	6
	ATOM	1990	N	ARG	A	260	51.088	4.696	-19.069	1.00	46.77	7
	ATOM	1991	CA	ARG	A	260	49.800	5.397	-19.104	1.00	45.39	6
	ATOM	1992	C	ARG	A	260	49.991	6.882	-19.278	1.00	41.75	6
20	ATOM	1993	O	ARG	A	260	50.970	7.421	-18.763	1.00	41.96	8
	ATOM	1994	CB	ARG	A	260	49.004	5.146	-17.814	1.00	48.72	6
	ATOM	1995	CG	ARG	A	260	48.340	3.797	-17.715	1.00	52.78	6
	ATOM	1996	CD	ARG	A	260	47.783	3.490	-16.342	1.00	56.11	6
	ATOM	1997	NE	ARG	A	260	48.800	3.016	-15.423	1.00	60.02	7
25	ATOM	1998	CZ	ARG	A	260	49.366	1.817	-15.362	1.00	61.86	6
	ATOM	1999	NH1	ARG	A	260	49.066	0.806	-16.179	1.00	62.97	7
	ATOM	2000	NH2	ARG	A	260	50.275	1.615	-14.410	1.00	62.19	7
	ATOM	2001	N	ALA	A	261	49.079	7.547	-20.024	1.00	39.42	7
	ATOM	2002	CA	ALA	A	261	49.232	8.993	-20.107	1.00	35.31	6
30	ATOM	2003	C	ALA	A	261	47.928	9.630	-19.612	1.00	32.26	6
	ATOM	2004	O	ALA	A	261	46.872	9.005	-19.790	1.00	34.66	8
	ATOM	2005	CB	ALA	A	261	49.538	9.504	-21.504	1.00	34.95	6
	ATOM	2006	N	VAL	A	262	48.060	10.831	-19.087	1.00	29.67	7
	ATOM	2007	CA	VAL	A	262	46.852	11.578	-18.705	1.00	27.51	6
35	ATOM	2008	C	VAL	A	262	46.916	12.796	-19.608	1.00	27.97	6
	ATOM	2009	O	VAL	A	262	47.977	13.414	-19.791	1.00	26.28	8
	ATOM	2010	CB	VAL	A	262	46.750	11.979	-17.233	1.00	29.25	6
	ATOM	2011	CG1	VAL	A	262	47.995	12.725	-16.785	1.00	30.58	6
	ATOM	2012	CG2	VAL	A	262	45.527	12.884	-16.976	1.00	30.36	6
40	ATOM	2013	N	ILE	A	263	45.801	13.185	-20.185	1.00	26.21	7
	ATOM	2014	CA	ILE	A	263	45.639	14.343	-21.031	1.00	26.33	6
	ATOM	2015	C	ILE	A	263	44.738	15.341	-20.300	1.00	28.09	6
	ATOM	2016	O	ILE	A	263	43.635	14.903	-19.935	1.00	26.14	8
	ATOM	2017	CB	ILE	A	263	44.977	13.970	-22.357	1.00	27.18	6
45	ATOM	2018	CG1	ILE	A	263	45.701	12.767	-22.999	1.00	30.42	6
	ATOM	2019	CG2	ILE	A	263	44.931	15.184	-23.302	1.00	26.41	6
	ATOM	2020	CD1	ILE	A	263	44.751	11.943	-23.867	1.00	32.55	6
	ATOM	2021	N	LEU	A	264	45.198	16.564	-20.149	1.00	28.73	7
	ATOM	2022	CA	LEU	A	264	44.453	17.626	-19.514	1.00	30.58	6
50	ATOM	2023	C	LEU	A	264	44.108	18.698	-20.530	1.00	29.44	6
	ATOM	2024	O	LEU	A	264	45.005	19.177	-21.235	1.00	30.50	8
	ATOM	2025	CB	LEU	A	264	45.273	18.264	-18.392	1.00	33.45	6
	ATOM	2026	CG	LEU	A	264	46.310	17.397	-17.677	1.00	35.36	6
	ATOM	2027	CD1	LEU	A	264	47.287	18.261	-16.855	1.00	38.43	6
55	ATOM	2028	CD2	LEU	A	264	45.634	16.357	-16.800	1.00	36.22	6
	ATOM	2029	N	VAL	A	265	42.875	19.166	-20.643	1.00	28.12	7
	ATOM	2030	CA	VAL	A	265	42.516	20.228	-21.586	1.00	30.77	6
	ATOM	2031	C	VAL	A	265	41.662	21.288	-20.868	1.00	30.38	6
	ATOM	2032	O	VAL	A	265	40.888	20.946	-19.964	1.00	33.23	8
60	ATOM	2033	CB	VAL	A	265	41.740	19.716	-22.798	1.00	30.45	6
	ATOM	2034	CG1	VAL	A	265	42.546	18.732	-23.649	1.00	31.64	6
	ATOM	2035	CG2	VAL	A	265	40.456	18.962	-22.415	1.00	30.65	6
	ATOM	2036	N	ALA	A	266	41.822	22.538	-21.233	1.00	30.29	7
	ATOM	2037	CA	ALA	A	266	40.992	23.628	-20.697	1.00	27.93	6
65	ATOM	2038	C	ALA	A	266	40.722	24.514	-21.890	1.00	28.75	6
	ATOM	2039	O	ALA	A	266	41.687	24.771	-22.653	1.00	31.65	8
	ATOM	2040	CB	ALA	A	266	41.637	24.388	-19.574	1.00	28.93	6
	ATOM	2041	N	ALA	A	267	39.535	25.012	-22.069	1.00	27.14	7
	ATOM	2042	CA	ALA	A	267	39.237	25.880	-23.189	1.00	28.13	6
70	ATOM	2043	C	ALA	A	267	38.051	26.744	-22.796	1.00	29.67	6
	ATOM	2044	O	ALA	A	267	37.054	26.257	-22.261	1.00	27.60	8
	ATOM	2045	CB	ALA	A	267	38.861	25.167	-24.478	1.00	26.05	6
	ATOM	2046	N	TRP	A	268	38.151	28.007	-23.166	1.00	29.63	7
	ATOM	2047	CA	TRP	A	268	37.074	28.951	-22.969	1.00	28.26	6
	ATOM	2048	C	TRP	A	268	36.049	28.766	-24.072	1.00	29.88	6

-64-

	ATOM	2049	O	TRP	A	268	36.407	28.609	-25.245	1.00	30.20	8
	ATOM	2050	CB	TRP	A	268	37.599	30.394	-22.996	1.00	30.40	6
	ATOM	2051	CG	TRP	A	268	38.406	30.735	-21.778	1.00	31.50	6
5	ATOM	2052	CD1	TRP	A	268	39.756	30.638	-21.572	1.00	32.04	6
	ATOM	2053	CD2	TRP	A	268	37.850	31.336	-20.602	1.00	29.94	6
	ATOM	2054	NE1	TRP	A	268	40.071	31.097	-20.307	1.00	32.09	7
	ATOM	2055	CE2	TRP	A	268	38.905	31.521	-19.699	1.00	32.20	6
	ATOM	2056	CE3	TRP	A	268	36.543	31.660	-20.214	1.00	29.41	6
10	ATOM	2057	CZ2	TRP	A	268	38.729	32.062	-18.420	1.00	30.97	6
	ATOM	2058	CZ3	TRP	A	268	36.362	32.188	-18.965	1.00	30.37	6
	ATOM	2059	CH2	TRP	A	268	37.448	32.390	-18.097	1.00	29.74	6
	ATOM	2060	N	LEU	A	269	34.789	28.947	-23.715	1.00	28.17	7
	ATOM	2061	CA	LEU	A	269	33.648	28.954	-24.579	1.00	29.03	6
15	ATOM	2062	C	LEU	A	269	32.680	29.913	-23.885	1.00	29.91	6
	ATOM	2063	O	LEU	A	269	32.201	29.674	-22.758	1.00	25.57	8
	ATOM	2064	CB	LEU	A	269	33.139	27.528	-24.786	1.00	30.48	6
	ATOM	2065	CG	LEU	A	269	31.952	27.443	-25.719	1.00	31.96	6
	ATOM	2066	CD1	LEU	A	269	32.337	27.993	-27.103	1.00	30.89	6
20	ATOM	2067	CD2	LEU	A	269	31.423	26.003	-25.790	1.00	31.19	6
	ATOM	2068	N	GLY	A	270	32.559	31.132	-24.446	1.00	29.19	7
	ATOM	2069	CA	GLY	A	270	31.738	32.156	-23.798	1.00	29.83	6
	ATOM	2070	C	GLY	A	270	32.341	32.563	-22.463	1.00	32.39	6
	ATOM	2071	O	GLY	A	270	33.549	32.829	-22.369	1.00	32.69	8
25	ATOM	2072	N	ASP	A	271	31.552	32.562	-21.390	1.00	30.56	7
	ATOM	2073	CA	ASP	A	271	32.088	32.888	-20.075	1.00	31.93	6
	ATOM	2074	C	ASP	A	271	32.450	31.649	-19.271	1.00	31.25	6
	ATOM	2075	O	ASP	A	271	32.749	31.710	-18.079	1.00	30.60	8
	ATOM	2076	CB	ASP	A	271	31.087	33.758	-19.289	1.00	33.98	6
30	ATOM	2077	CG	ASP	A	271	31.073	35.165	-19.921	1.00	37.85	6
	ATOM	2078	OD1	ASP	A	271	32.103	35.682	-20.401	1.00	38.52	8
	ATOM	2079	OD2	ASP	A	271	29.996	35.770	-19.944	1.00	39.53	8
	ATOM	2080	N	ALA	A	272	32.462	30.482	-19.903	1.00	29.77	7
	ATOM	2081	CA	ALA	A	272	32.828	29.254	-19.228	1.00	27.77	6
35	ATOM	2082	C	ALA	A	272	34.256	28.826	-19.557	1.00	26.45	6
	ATOM	2083	O	ALA	A	272	34.545	28.837	-20.745	1.00	26.44	8
	ATOM	2084	CB	ALA	A	272	31.977	28.068	-19.666	1.00	27.56	6
	ATOM	2085	N	ARG	A	273	35.053	28.448	-18.602	1.00	25.11	7
	ATOM	2086	CA	ARG	A	273	36.354	27.839	-18.859	1.00	25.96	6
40	ATOM	2087	C	ARG	A	273	36.194	26.346	-18.606	1.00	23.79	6
	ATOM	2088	O	ARG	A	273	36.292	25.868	-17.465	1.00	25.36	8
	ATOM	2089	CB	ARG	A	273	37.467	28.400	-17.962	1.00	27.51	6
	ATOM	2090	CG	ARG	A	273	38.864	27.853	-18.355	1.00	27.52	6
	ATOM	2091	CD	ARG	A	273	39.848	28.605	-17.421	1.00	28.40	6
45	ATOM	2092	NE	ARG	A	273	41.215	28.212	-17.720	0.50	26.25	7
	ATOM	2093	CZ	ARG	A	273	41.850	27.144	-17.306	0.50	26.10	6
	ATOM	2094	NH1	ARG	A	273	41.229	26.281	-16.517	0.50	28.04	7
	ATOM	2095	NH2	ARG	A	273	43.107	26.909	-17.691	0.50	25.33	7
	ATOM	2096	N	LEU	A	274	35.918	25.587	-19.693	1.00	25.09	7
50	ATOM	2097	CA	LEU	A	274	35.608	24.173	-19.545	1.00	23.10	6
	ATOM	2098	C	LEU	A	274	36.845	23.385	-19.359	1.00	23.02	6
	ATOM	2099	O	LEU	A	274	37.846	23.706	-20.001	1.00	24.38	8
	ATOM	2100	CB	LEU	A	274	34.863	23.714	-20.847	1.00	22.40	6
	ATOM	2101	CG	LEU	A	274	33.548	24.488	-21.045	1.00	22.92	6
55	ATOM	2102	CD1	LEU	A	274	32.953	24.119	-22.368	1.00	25.59	6
	ATOM	2103	CD2	LEU	A	274	32.619	24.185	-19.846	1.00	24.66	6
	ATOM	2104	N	ILE	A	275	36.844	22.342	-18.576	1.00	22.01	7
	ATOM	2105	CA	ILE	A	275	37.965	21.529	-18.235	1.00	24.38	6
	ATOM	2106	C	ILE	A	275	37.640	20.072	-18.439	1.00	24.31	6
60	ATOM	2107	O	ILE	A	275	36.504	19.675	-18.126	1.00	23.32	8
	ATOM	2108	CB	ILE	A	275	38.290	21.785	-16.743	1.00	27.33	6
	ATOM	2109	CG1	ILE	A	275	38.853	23.233	-16.577	1.00	30.12	6
	ATOM	2110	CG2	ILE	A	275	39.295	20.826	-16.161	1.00	32.15	6
	ATOM	2111	CD1	ILE	A	275	38.634	23.632	-15.112	1.00	33.95	6
65	ATOM	2112	N	ASP	A	276	38.611	19.282	-18.865	1.00	23.56	7
	ATOM	2113	CA	ASP	A	276	38.347	17.845	-19.005	1.00	24.73	6
	ATOM	2114	C	ASP	A	276	39.702	17.125	-18.966	1.00	24.26	6
	ATOM	2115	O	ASP	A	276	40.768	17.741	-19.153	1.00	24.98	8
	ATOM	2116	CB	ASP	A	276	37.551	17.545	-20.271	1.00	24.30	6
	ATOM	2117	CG	ASP	A	276	36.730	16.276	-20.290	1.00	26.28	6
70	ATOM	2118	OD1	ASP	A	276	36.927	15.468	-19.324	1.00	27.91	8
	ATOM	2119	OD2	ASP	A	276	35.946	16.119	-21.251	1.00	25.73	8
	ATOM	2120	N	ASN	A	277	39.671	15.855	-18.697	1.00	22.14	7
	ATOM	2121	CA	ASN	A	277	40.857	15.020	-18.682	1.00	25.69	6
	ATOM	2122	C	ASN	A	277	40.473	13.587	-19.027	1.00	24.93	6

-65-

5	ATOM	2123	O	ASN A 277	39.335	13.139	-18.920	1.00	25.86	8
	ATOM	2124	CB	ASN A 277	41.608	15.073	-17.350	1.00	28.42	6
	ATOM	2125	CG	ASN A 277	41.077	14.298	-16.164	1.00	32.43	6
	ATOM	2126	OD1	ASN A 277	40.715	13.140	-16.247	1.00	37.45	8
	ATOM	2127	ND2	ASN A 277	41.023	14.889	-14.994	1.00	35.65	7
	ATOM	2128	N	LYS A 278	41.517	12.825	-19.428	1.00	28.31	7
	ATOM	2129	CA	LYS A 278	41.338	11.429	-19.765	1.00	31.78	6
	ATOM	2130	C	LYS A 278	42.655	10.677	-19.634	1.00	33.11	6
10	ATOM	2131	O	LYS A 278	43.692	11.227	-19.991	1.00	33.12	8
	ATOM	2132	CB	LYS A 278	40.814	11.323	-21.189	1.00	32.53	6
	ATOM	2133	CG	LYS A 278	40.748	10.008	-21.905	1.00	35.09	6
	ATOM	2134	CD	LYS A 278	39.814	10.144	-23.124	1.00	38.06	6
	ATOM	2135	CE	LYS A 278	39.115	8.808	-23.384	1.00	39.45	6
	ATOM	2136	NZ	LYS A 278	37.984	9.018	-24.354	1.00	40.81	7
15	ATOM	2137	N	MET A 279	42.594	9.455	-19.139	1.00	35.39	7
	ATOM	2138	CA	MET A 279	43.799	8.636	-19.046	1.00	39.07	6
	ATOM	2139	C	MET A 279	43.777	7.645	-20.201	1.00	40.75	6
	ATOM	2140	O	MET A 279	42.688	7.224	-20.590	1.00	39.38	8
20	ATOM	2141	CB	MET A 279	43.895	7.997	-17.641	1.00	42.09	6
	ATOM	2142	CG	MET A 279	44.366	9.076	-16.657	1.00	45.36	6
	ATOM	2143	SD	MET A 279	44.591	8.656	-14.926	1.00	51.28	16
	ATOM	2144	CE	MET A 279	42.948	8.136	-14.428	1.00	49.74	6
	ATOM	2145	N	VAL A 280	44.953	7.391	-20.786	1.00	41.33	7
25	ATOM	2146	CA	VAL A 280	44.994	6.466	-21.917	1.00	44.04	6
	ATOM	2147	C	VAL A 280	46.138	5.483	-21.692	1.00	45.91	6
	ATOM	2148	O	VAL A 280	47.232	5.881	-21.274	1.00	44.69	8
	ATOM	2149	CB	VAL A 280	45.126	7.195	-23.265	1.00	43.07	6
	ATOM	2150	CG1	VAL A 280	46.430	7.978	-23.326	1.00	43.41	6
30	ATOM	2151	CG2	VAL A 280	45.060	6.239	-24.439	1.00	43.94	6
	ATOM	2152	N	GLU A 281	45.787	4.211	-21.867	1.00	51.13	7
	ATOM	2153	CA	GLU A 281	46.797	3.151	-21.712	1.00	54.78	6
	ATOM	2154	C	GLU A 281	47.658	3.176	-22.971	1.00	55.75	6
	ATOM	2155	O	GLU A 281	47.155	3.235	-24.094	1.00	55.40	8
35	ATOM	2156	CB	GLU A 281	46.186	1.784	-21.469	1.00	56.82	6
	ATOM	2157	CG	GLU A 281	45.244	1.658	-20.296	1.00	59.30	6
	ATOM	2158	CD	GLU A 281	45.898	1.424	-18.957	1.00	61.75	6
	ATOM	2159	OE1	GLU A 281	47.135	1.218	-18.919	1.00	62.80	8
	ATOM	2160	OE2	GLU A 281	45.187	1.411	-17.923	1.00	62.74	8
40	ATOM	2161	N	LEU A 282	48.958	3.235	-22.781	1.00	57.94	7
	ATOM	2162	CA	LEU A 282	49.944	3.334	-23.844	1.00	60.20	6
	ATOM	2163	C	LEU A 282	50.394	1.966	-24.343	1.00	62.75	6
	ATOM	2164	O	LEU A 282	50.792	1.813	-25.501	1.00	63.61	8
	ATOM	2165	CB	LEU A 282	51.132	4.160	-23.353	1.00	60.14	6
45	ATOM	2166	CG	LEU A 282	51.250	5.643	-23.655	1.00	59.64	6
	ATOM	2167	CD1	LEU A 282	49.954	6.281	-24.103	1.00	59.72	6
	ATOM	2168	CD2	LEU A 282	51.880	6.386	-22.494	1.00	58.92	6
	ATOM	2169	N	ALA A 283	50.285	0.961	-23.484	1.00	64.72	7
	ATOM	2170	CA	ALA A 283	50.637	-0.410	-23.818	1.00	66.41	6
50	ATOM	2171	C	ALA A 283	49.397	-1.291	-23.933	1.00	67.10	6
	ATOM	2172	O	ALA A 283	48.394	-0.879	-24.563	1.00	68.25	8
	ATOM	2173	CB	ALA A 283	51.563	-1.007	-22.764	1.00	66.62	6

55 Monomer B

			Atom type				X	Y	Z	Occ.	B	Atomic No.
60	ATOM	2174	N	MET	B	1	58.003	-23.593	11.263	1.00	36.48	7
	ATOM	2175	CA	MET	B	1	58.132	-22.126	11.083	1.00	33.40	6
	ATOM	2176	C	MET	B	1	58.194	-21.749	9.627	1.00	33.88	6
	ATOM	2177	O	MET	B	1	59.003	-22.271	8.843	1.00	34.96	8
65	ATOM	2178	CB	MET	B	1	59.383	-21.686	11.860	1.00	32.85	6
	ATOM	2179	CG	MET	B	1	59.602	-20.178	11.711	1.00	32.05	6
	ATOM	2180	SD	MET	B	1	61.001	-19.706	12.738	1.00	32.48	16
	ATOM	2181	CE	MET	B	1	62.316	-19.795	11.507	1.00	33.02	6
70	ATOM	2182	N	LEU	B	2	57.366	-20.850	9.145	1.00	30.67	7
	ATOM	2183	CA	LEU	B	2	57.332	-20.400	7.790	1.00	31.35	6
	ATOM	2184	C	LEU	B	2	58.315	-19.246	7.576	1.00	32.39	6
	ATOM	2185	O	LEU	B	2	58.367	-18.394	8.491	1.00	31.76	8
	ATOM	2186	CB	LEU	B	2	55.926	-19.896	7.473	1.00	35.48	6
	ATOM	2187	CG	LEU	B	2	54.773	-20.875	7.670	1.00	38.24	6
	ATOM	2188	CD1	LEU	B	2	53.410	-20.187	7.668	1.00	37.95	6

-66-

	ATOM	2189	CD2	LEU	B	2	54.803	-21.930	6.560	1.00	38.99	6
	ATOM	2190	N	ILE	B	3	58.980	-19.217	6.439	1.00	28.48	7
	ATOM	2191	CA	ILE	B	3	59.916	-18.162	6.099	1.00	29.00	6
5	ATOM	2192	C	ILE	B	3	59.442	-17.553	4.806	1.00	30.65	6
	ATOM	2193	O	ILE	B	3	59.350	-18.257	3.778	1.00	31.80	8
	ATOM	2194	CB	ILE	B	3	61.380	-18.634	5.938	1.00	31.56	6
	ATOM	2195	CG1	ILE	B	3	61.859	-19.222	7.261	1.00	31.29	6
	ATOM	2196	CG2	ILE	B	3	62.257	-17.481	5.477	1.00	32.77	6
10	ATOM	2197	CD1	ILE	B	3	63.283	-19.769	7.266	1.00	37.37	6
	ATOM	2198	N	ILE	B	4	58.918	-16.333	4.826	1.00	24.55	7
	ATOM	2199	CA	ILE	B	4	58.284	-15.663	3.748	1.00	26.13	6
	ATOM	2200	C	ILE	B	4	59.159	-14.534	3.279	1.00	28.00	6
	ATOM	2201	O	ILE	B	4	59.649	-13.738	4.079	1.00	28.39	8
15	ATOM	2202	CB	ILE	B	4	56.926	-15.034	4.179	1.00	26.38	6
	ATOM	2203	CG1	ILE	B	4	56.042	-16.103	4.827	1.00	30.33	6
	ATOM	2204	CG2	ILE	B	4	56.248	-14.318	3.013	1.00	28.07	6
	ATOM	2205	CD1	ILE	B	4	55.611	-17.272	3.955	1.00	30.56	6
	ATOM	2206	N	GLU	B	5	59.374	-14.485	1.987	1.00	29.37	7
20	ATOM	2207	CA	GLU	B	5	60.209	-13.449	1.380	1.00	31.10	6
	ATOM	2208	C	GLU	B	5	59.387	-12.614	0.487	1.00	30.29	6
	ATOM	2209	O	GLU	B	5	59.982	-11.574	0.059	1.00	32.17	8
	ATOM	2210	CB	GLU	B	5	61.292	-14.267	0.655	1.00	35.81	6
	ATOM	2211	CG	GLU	B	5	62.267	-15.017	1.547	1.00	40.51	6
25	ATOM	2212	CD	GLU	B	5	63.167	-15.907	0.709	1.00	45.93	6
	ATOM	2213	OE1	GLU	B	5	63.562	-16.994	1.195	1.00	48.88	8
	ATOM	2214	OE2	GLU	B	5	63.451	-15.521	-0.447	1.00	46.38	8
	ATOM	2215	N	THR	B	6	58.142	-12.721	0.076	1.00	26.13	7
	ATOM	2216	CA	THR	B	6	57.578	-11.758	-0.836	1.00	27.91	6
30	ATOM	2217	C	THR	B	6	56.298	-11.128	-0.207	1.00	24.93	6
	ATOM	2218	O	THR	B	6	55.656	-11.788	0.619	1.00	27.98	8
	ATOM	2219	CB	THR	B	6	57.229	-12.351	-2.205	1.00	31.04	6
	ATOM	2220	OG1	THR	B	6	56.159	-13.300	-2.052	1.00	30.86	8
	ATOM	2221	CG2	THR	B	6	58.425	-13.076	-2.851	1.00	31.94	6
35	ATOM	2222	N	LEU	B	7	55.927	-10.037	-0.790	1.00	27.39	7
	ATOM	2223	CA	LEU	B	7	54.715	-9.308	-0.367	1.00	28.55	6
	ATOM	2224	C	LEU	B	7	53.455	-10.153	-0.636	1.00	27.46	6
	ATOM	2225	O	LEU	B	7	52.669	-10.343	0.308	1.00	26.58	8
	ATOM	2226	CB	LEU	B	7	54.583	-7.921	-0.986	1.00	29.88	6
40	ATOM	2227	CG	LEU	B	7	55.750	-6.939	-0.729	1.00	31.25	6
	ATOM	2228	CD1	LEU	B	7	55.361	-5.499	-1.043	1.00	31.80	6
	ATOM	2229	CD2	LEU	B	7	56.271	-7.052	0.703	1.00	30.25	6
	ATOM	2230	N	PRO	B	8	53.288	-10.697	-1.811	1.00	28.20	7
	ATOM	2231	CA	PRO	B	8	52.092	-11.501	-2.092	1.00	28.01	6
45	ATOM	2232	C	PRO	B	8	51.973	-12.671	-1.172	1.00	27.27	6
	ATOM	2233	O	PRO	B	8	50.869	-12.943	-0.641	1.00	26.76	8
	ATOM	2234	CB	PRO	B	8	52.264	-11.941	-3.550	1.00	30.16	6
	ATOM	2235	CG	PRO	B	8	53.126	-10.877	-4.147	1.00	30.87	6
	ATOM	2236	CD	PRO	B	8	54.088	-10.500	-3.047	1.00	28.88	6
50	ATOM	2237	N	LEU	B	9	53.045	-13.427	-0.954	1.00	25.43	7
	ATOM	2238	CA	LEU	B	9	53.054	-14.599	-0.088	1.00	25.93	6
	ATOM	2239	C	LEU	B	9	52.839	-14.206	1.363	1.00	27.59	6
	ATOM	2240	O	LEU	B	9	52.069	-14.843	2.081	1.00	25.94	8
	ATOM	2241	CB	LEU	B	9	54.355	-15.416	-0.317	1.00	27.71	6
55	ATOM	2242	CG	LEU	B	9	54.311	-16.200	-1.656	1.00	31.97	6
	ATOM	2243	CD1	LEU	B	9	55.671	-16.790	-1.961	1.00	30.14	6
	ATOM	2244	CD2	LEU	B	9	53.236	-17.279	-1.607	1.00	32.64	6
	ATOM	2245	N	LEU	B	10	53.323	-13.028	1.819	1.00	25.26	7
	ATOM	2246	CA	LEU	B	10	53.068	-12.583	3.182	1.00	23.45	6
60	ATOM	2247	C	LEU	B	10	51.581	-12.234	3.362	1.00	22.04	6
	ATOM	2248	O	LEU	B	10	50.941	-12.683	4.336	1.00	22.46	8
	ATOM	2249	CB	LEU	B	10	53.963	-11.368	3.535	1.00	25.32	6
	ATOM	2250	CG	LEU	B	10	53.618	-10.738	4.917	1.00	23.24	6
	ATOM	2251	CD1	LEU	B	10	53.904	-11.665	6.068	1.00	21.41	6
65	ATOM	2252	CD2	LEU	B	10	54.376	-9.417	5.105	1.00	22.97	6
	ATOM	2253	N	ARG	B	11	50.992	-11.537	2.407	1.00	23.80	7
	ATOM	2254	CA	ARG	B	11	49.591	-11.130	2.459	1.00	26.88	6
	ATOM	2255	C	ARG	B	11	48.681	-12.350	2.583	1.00	26.18	6
	ATOM	2256	O	ARG	B	11	47.707	-12.322	3.328	1.00	23.87	8
70	ATOM	2257	CB	ARG	B	11	49.208	-10.303	1.232	1.00	26.73	6
	ATOM	2258	CG	ARG	B	11	49.968	-8.984	1.209	1.00	29.98	6
	ATOM	2259	CD	ARG	B	11	49.306	-7.986	0.278	1.00	35.78	6
	ATOM	2260	NE	ARG	B	11	49.673	-6.602	0.492	1.00	38.73	7
	ATOM	2261	CZ	ARG	B	11	50.447	-5.830	-0.254	1.00	39.79	6
	ATOM	2262	NH1	ARG	B	11	51.031	-6.255	-1.376	1.00	41.64	7

-67-

	ATOM	2263	NH2	ARG	B	11	50.651	-4.546	0.070	1.00	40.26	7
	ATOM	2264	N	GLN	B	12	48.992	-13.409	1.864	1.00	24.75	7
	ATOM	2265	CA	GLN	B	12	48.289	-14.712	1.885	1.00	23.93	6
5	ATOM	2266	C	GLN	B	12	48.282	-15.281	3.285	1.00	23.24	6
	ATOM	2267	O	GLN	B	12	47.231	-15.711	3.804	1.00	23.11	8
	ATOM	2268	CB	GLN	B	12	48.919	-15.669	0.879	1.00	25.20	6
	ATOM	2269	CG	GLN	B	12	48.494	-17.114	0.983	1.00	31.10	6
	ATOM	2270	CD	GLN	B	12	48.983	-18.004	-0.160	1.00	33.85	6
10	ATOM	2271	OE1	GLN	B	12	50.160	-18.359	-0.226	1.00	34.46	8
	ATOM	2272	NE2	GLN	B	12	48.024	-18.373	-1.035	1.00	37.05	7
	ATOM	2273	N	GLN	B	13	49.406	-15.241	4.018	1.00	20.76	7
	ATOM	2274	CA	GLN	B	13	49.531	-15.725	5.367	1.00	21.58	6
	ATOM	2275	C	GLN	B	13	48.755	-14.802	6.342	1.00	19.88	6
15	ATOM	2276	O	GLN	B	13	48.070	-15.312	7.250	1.00	20.12	8
	ATOM	2277	CB	GLN	B	13	51.005	-15.852	5.844	1.00	22.55	6
	ATOM	2278	CG	GLN	B	13	51.779	-16.951	5.087	1.00	25.94	6
	ATOM	2279	CD	GLN	B	13	51.107	-18.297	5.150	1.00	27.86	6
	ATOM	2280	OE1	GLN	B	13	50.677	-18.693	6.225	1.00	28.91	8
20	ATOM	2281	NE2	GLN	B	13	50.985	-18.937	3.993	1.00	32.63	7
	ATOM	2282	N	ILE	B	14	48.738	-13.510	6.042	1.00	21.05	7
	ATOM	2283	CA	ILE	B	14	48.035	-12.575	6.947	1.00	20.18	6
	ATOM	2284	C	ILE	B	14	46.501	-12.822	6.819	1.00	21.51	6
	ATOM	2285	O	ILE	B	14	45.800	-12.838	7.850	1.00	21.76	8
25	ATOM	2286	CB	ILE	B	14	48.438	-11.133	6.718	1.00	21.52	6
	ATOM	2287	CG1	ILE	B	14	49.931	-10.873	7.014	1.00	21.53	6
	ATOM	2288	CG2	ILE	B	14	47.609	-10.137	7.572	1.00	20.30	6
	ATOM	2289	CD1	ILE	B	14	50.448	-11.493	8.287	1.00	20.36	6
	ATOM	2290	N	ARG	B	15	46.060	-13.042	5.580	1.00	21.97	7
30	ATOM	2291	CA	ARG	B	15	44.640	-13.407	5.403	1.00	21.03	6
	ATOM	2292	C	ARG	B	15	44.328	-14.704	6.120	1.00	20.84	6
	ATOM	2293	O	ARG	B	15	43.231	-14.819	6.693	1.00	21.21	8
	ATOM	2294	CB	ARG	B	15	44.362	-13.468	3.903	1.00	23.95	6
	ATOM	2295	CG	ARG	B	15	44.439	-12.110	3.182	1.00	28.33	6
35	ATOM	2296	CD	ARG	B	15	43.633	-12.304	1.885	1.00	35.29	6
	ATOM	2297	NE	ARG	B	15	44.463	-13.095	0.938	1.00	39.61	7
	ATOM	2298	CZ	ARG	B	15	45.378	-12.352	0.272	1.00	43.48	6
	ATOM	2299	NH1	ARG	B	15	45.533	-11.036	0.426	1.00	44.40	7
	ATOM	2300	NH2	ARG	B	15	46.158	-12.973	-0.594	1.00	43.72	7
40	ATOM	2301	N	ARG	B	16	45.189	-15.724	6.069	1.00	18.66	7
	ATOM	2302	CA	ARG	B	16	44.923	-16.986	6.717	1.00	19.99	6
	ATOM	2303	C	ARG	B	16	44.816	-16.743	8.234	1.00	20.42	6
	ATOM	2304	O	ARG	B	16	43.855	-17.229	8.824	1.00	19.70	8
	ATOM	2305	CB	ARG	B	16	45.959	-18.073	6.435	1.00	22.24	6
45	ATOM	2306	CG	ARG	B	16	45.869	-19.264	7.352	1.00	23.29	6
	ATOM	2307	CD	ARG	B	16	46.986	-20.277	7.132	1.00	25.24	6
	ATOM	2308	NE	ARG	B	16	48.309	-19.702	7.470	1.00	27.88	7
	ATOM	2309	CZ	ARG	B	16	48.797	-19.716	8.706	1.00	28.92	6
	ATOM	2310	NH1	ARG	B	16	50.016	-19.215	8.961	1.00	28.52	7
50	ATOM	2311	NH2	ARG	B	16	48.126	-20.327	9.679	1.00	24.92	7
	ATOM	2312	N	LEU	B	17	45.716	-15.933	8.815	1.00	19.27	7
	ATOM	2313	CA	LEU	B	17	45.626	-15.699	10.270	1.00	20.77	6
	ATOM	2314	C	LEU	B	17	44.352	-14.990	10.702	1.00	20.30	6
	ATOM	2315	O	LEU	B	17	43.778	-15.286	11.759	1.00	19.03	8
55	ATOM	2316	CB	LEU	B	17	46.900	-14.923	10.697	1.00	22.28	6
	ATOM	2317	CG	LEU	B	17	48.154	-15.834	10.589	1.00	20.91	6
	ATOM	2318	CD1	LEU	B	17	49.346	-14.854	10.747	1.00	23.26	6
	ATOM	2319	CD2	LEU	B	17	48.210	-16.976	11.546	1.00	23.26	6
	ATOM	2320	N	ARG	B	18	43.880	-14.084	9.852	1.00	20.08	7
60	ATOM	2321	CA	ARG	B	18	42.616	-13.394	10.085	1.00	20.19	6
	ATOM	2322	C	ARG	B	18	41.443	-14.367	10.053	1.00	20.24	6
	ATOM	2323	O	ARG	B	18	40.595	-14.419	10.938	1.00	19.77	8
	ATOM	2324	CB	ARG	B	18	42.410	-12.287	9.049	1.00	19.52	6
	ATOM	2325	CG	ARG	B	18	41.388	-11.239	9.456	1.00	25.28	6
65	ATOM	2326	CD	ARG	B	18	40.953	-10.402	8.264	1.00	30.78	6
	ATOM	2327	NE	ARG	B	18	42.033	-9.556	7.766	1.00	37.79	7
	ATOM	2328	CZ	ARG	B	18	42.285	-9.348	6.478	1.00	41.34	6
	ATOM	2329	NH1	ARG	B	18	41.532	-9.927	5.553	1.00	41.84	7
	ATOM	2330	NH2	ARG	B	18	43.290	-8.562	6.119	1.00	42.14	7
70	ATOM	2331	N	MET	B	19	41.447	-15.266	9.053	1.00	19.56	7
	ATOM	2332	CA	MET	B	19	40.384	-16.272	8.983	1.00	21.07	6
	ATOM	2333	C	MET	B	19	40.376	-17.192	10.199	1.00	19.93	6
	ATOM	2334	O	MET	B	19	39.291	-17.611	10.629	1.00	18.95	8
	ATOM	2335	CB	MET	B	19	40.507	-17.047	7.683	1.00	21.11	6
	ATOM	2336	CG	MET	B	19	39.650	-18.307	7.449	1.00	22.70	6

-68-

	ATOM	2337	SD	MET	B	19	40.253	-19.824	8.206	1.00	21.29	16
	ATOM	2338	CE	MET	B	19	41.816	-20.143	7.368	1.00	22.90	6
	ATOM	2339	N	GLU	B	20	41.516	-17.512	10.731	1.00	18.16	7
5	ATOM	2340	CA	GLU	B	20	41.687	-18.429	11.858	1.00	20.12	6
	ATOM	2341	C	GLU	B	20	41.280	-17.732	13.182	1.00	20.85	6
	ATOM	2342	O	GLU	B	20	41.156	-18.387	14.243	1.00	24.28	8
	ATOM	2343	CB	GLU	B	20	43.113	-18.960	11.945	1.00	18.82	6
	ATOM	2344	CG	GLU	B	20	43.467	-19.977	10.846	1.00	21.83	6
10	ATOM	2345	CD	GLU	B	20	44.911	-20.433	10.890	1.00	26.79	6
	ATOM	2346	OE1	GLU	B	20	45.611	-20.063	11.869	1.00	28.93	8
	ATOM	2347	OE2	GLU	B	20	45.312	-21.210	9.985	1.00	26.44	8
	ATOM	2348	N	GLY	B	21	41.236	-16.424	13.172	1.00	21.16	7
	ATOM	2349	CA	GLY	B	21	40.877	-15.568	14.299	1.00	20.08	6
15	ATOM	2350	C	GLY	B	21	42.055	-15.540	15.311	1.00	21.45	6
	ATOM	2351	O	GLY	B	21	41.856	-15.580	16.546	1.00	20.95	8
	ATOM	2352	N	LYS	B	22	43.279	-15.515	14.815	1.00	17.96	7
	ATOM	2353	CA	LYS	B	22	44.458	-15.503	15.668	1.00	21.37	6
	ATOM	2354	C	LYS	B	22	44.924	-14.091	15.953	1.00	23.78	6
20	ATOM	2355	O	LYS	B	22	44.942	-13.267	15.041	1.00	24.76	8
	ATOM	2356	CB	LYS	B	22	45.638	-16.191	14.984	1.00	22.71	6
	ATOM	2357	CG	LYS	B	22	45.420	-17.662	14.646	1.00	25.81	6
	ATOM	2358	CD	LYS	B	22	45.337	-18.553	15.836	1.00	28.29	6
	ATOM	2359	CE	LYS	B	22	44.963	-19.997	15.550	1.00	33.33	6
25	ATOM	2360	NZ	LYS	B	22	45.832	-20.715	14.575	1.00	29.69	7
	ATOM	2361	N	ARG	B	23	45.285	-13.775	17.175	1.00	19.63	7
	ATOM	2362	CA	ARG	B	23	45.917	-12.467	17.446	1.00	22.19	6
	ATOM	2363	C	ARG	B	23	47.415	-12.521	17.203	1.00	20.99	6
	ATOM	2364	O	ARG	B	23	48.014	-13.529	17.533	1.00	22.27	8
30	ATOM	2365	CB	ARG	B	23	45.620	-12.042	18.877	1.00	23.98	6
	ATOM	2366	CG	ARG	B	23	44.149	-11.748	19.161	1.00	33.05	6
	ATOM	2367	CD	ARG	B	23	43.965	-11.207	20.600	1.00	35.95	6
	ATOM	2368	NE	ARG	B	23	44.774	-11.865	21.560	1.00	39.00	7
	ATOM	2369	CZ	ARG	B	23	45.045	-12.903	22.319	1.00	38.30	6
35	ATOM	2370	NH1	ARG	B	23	44.343	-14.060	22.457	1.00	34.37	7
	ATOM	2371	NH2	ARG	B	23	46.204	-12.653	22.881	1.00	33.10	7
	ATOM	2372	N	VAL	B	24	47.873	-11.534	16.444	1.00	19.44	7
	ATOM	2373	CA	VAL	B	24	49.260	-11.534	15.984	1.00	19.87	6
	ATOM	2374	C	VAL	B	24	50.133	-10.493	16.615	1.00	20.77	6
40	ATOM	2375	O	VAL	B	24	49.724	-9.356	16.770	1.00	20.17	8
	ATOM	2376	CB	VAL	B	24	49.220	-11.301	14.473	1.00	20.82	6
	ATOM	2377	CG1	VAL	B	24	50.587	-11.071	13.856	1.00	21.58	6
	ATOM	2378	CG2	VAL	B	24	48.493	-12.516	13.838	1.00	22.44	6
	ATOM	2379	N	ALA	B	25	51.327	-10.950	17.072	1.00	18.32	7
45	ATOM	2380	CA	ALA	B	25	52.294	-9.989	17.591	1.00	18.65	6
	ATOM	2381	C	ALA	B	25	53.431	-9.885	16.600	1.00	22.09	6
	ATOM	2382	O	ALA	B	25	53.908	-10.915	16.053	1.00	26.60	8
	ATOM	2383	CB	ALA	B	25	52.871	-10.371	18.953	1.00	20.06	6
	ATOM	2384	N	LEU	B	26	53.922	-8.705	16.329	1.00	18.28	7
50	ATOM	2385	CA	LEU	B	26	54.997	-8.468	15.410	1.00	16.76	6
	ATOM	2386	C	LEU	B	26	56.273	-8.010	16.156	1.00	20.96	6
	ATOM	2387	O	LEU	B	26	56.139	-7.157	17.020	1.00	21.27	8
	ATOM	2388	CB	LEU	B	26	54.673	-7.425	14.340	1.00	19.09	6
	ATOM	2389	CG	LEU	B	26	55.816	-6.890	13.487	1.00	19.40	6
55	ATOM	2390	CD1	LEU	B	26	56.464	-7.969	12.603	1.00	21.45	6
	ATOM	2391	CD2	LEU	B	26	55.320	-5.738	12.604	1.00	22.40	6
	ATOM	2392	N	VAL	B	27	57.396	-8.642	15.874	1.00	20.49	7
	ATOM	2393	CA	VAL	B	27	58.684	-8.136	16.430	1.00	19.53	6
	ATOM	2394	C	VAL	B	27	59.576	-7.694	15.308	1.00	21.55	6
60	ATOM	2395	O	VAL	B	27	60.170	-8.516	14.520	1.00	22.20	8
	ATOM	2396	CB	VAL	B	27	59.378	-9.239	17.253	1.00	21.88	6
	ATOM	2397	CG1	VAL	B	27	60.658	-8.617	17.884	1.00	21.20	6
	ATOM	2398	CG2	VAL	B	27	58.513	-9.837	18.318	1.00	20.54	6
	ATOM	2399	N	PRO	B	28	59.761	-6.435	14.910	1.00	20.58	7
65	ATOM	2400	CA	PRO	B	28	60.557	-5.881	13.878	1.00	21.31	6
	ATOM	2401	C	PRO	B	28	62.068	-5.886	14.202	1.00	24.78	6
	ATOM	2402	O	PRO	B	28	62.428	-5.538	15.336	1.00	26.50	8
	ATOM	2403	CB	PRO	B	28	60.112	-4.424	13.720	1.00	22.66	6
	ATOM	2404	CG	PRO	B	28	58.741	-4.426	14.395	1.00	20.85	6
70	ATOM	2405	CD	PRO	B	28	58.946	-5.327	15.578	1.00	20.40	6
	ATOM	2406	N	THR	B	29	62.875	-6.483	13.317	1.00	26.26	7
	ATOM	2407	CA	THR	B	29	64.329	-6.556	13.614	1.00	25.08	6
	ATOM	2408	C	THR	B	29	65.126	-6.328	12.359	1.00	25.98	6
	ATOM	2409	O	THR	B	29	64.643	-6.415	11.228	1.00	23.47	8
	ATOM	2410	CB	THR	B	29	64.820	-7.900	14.201	1.00	26.97	6

-69-

	ATOM	2411	OG1	THR	B	29	65.022	-8.817	13.088	1.00	26.74	8
	ATOM	2412	CG2	THR	B	29	63.914	-8.579	15.219	1.00	25.95	6
	ATOM	2413	N	MET	B	30	66.471	-6.078	12.560	1.00	25.32	7
	ATOM	2414	CA	MET	B	30	67.357	-5.995	11.415	1.00	26.82	6
5	ATOM	2415	C	MET	B	30	68.261	-7.249	11.384	1.00	28.96	6
	ATOM	2416	O	MET	B	30	69.347	-7.183	10.815	1.00	30.56	8
	ATOM	2417	CB	MET	B	30	68.229	-4.738	11.416	1.00	26.43	6
	ATOM	2418	CG	MET	B	30	67.252	-3.504	11.203	1.00	27.24	6
10	ATOM	2419	SD	MET	B	30	67.969	-2.187	10.263	1.00	28.19	16
	ATOM	2420	CE	MET	B	30	69.323	-1.713	11.388	1.00	33.08	6
	ATOM	2421	N	GLY	B	31	67.793	-8.340	11.934	1.00	27.82	7
	ATOM	2422	CA	GLY	B	31	68.599	-9.593	11.926	1.00	29.40	6
	ATOM	2423	C	GLY	B	31	69.833	-9.495	12.829	1.00	31.29	6
15	ATOM	2424	O	GLY	B	31	69.934	-8.645	13.713	1.00	28.83	8
	ATOM	2425	N	ASN	B	32	70.728	-10.486	12.690	1.00	31.40	7
	ATOM	2426	CA	ASN	B	32	71.923	-10.565	13.552	1.00	33.60	6
	ATOM	2427	C	ASN	B	32	71.454	-10.664	14.982	1.00	30.00	6
	ATOM	2428	O	ASN	B	32	71.870	-9.961	15.906	1.00	32.23	8
20	ATOM	2429	CB	ASN	B	32	72.857	-9.379	13.347	1.00	35.71	6
	ATOM	2430	CG	ASN	B	32	74.231	-9.610	13.979	1.00	39.99	6
	ATOM	2431	OD1	ASN	B	32	74.920	-8.633	14.294	1.00	42.85	8
	ATOM	2432	ND2	ASN	B	32	74.607	-10.864	14.228	1.00	40.08	7
	ATOM	2433	N	LEU	B	33	70.506	-11.572	15.191	1.00	30.19	7
25	ATOM	2434	CA	LEU	B	33	69.833	-11.774	16.449	1.00	29.02	6
	ATOM	2435	C	LEU	B	33	70.684	-12.343	17.566	1.00	35.03	6
	ATOM	2436	O	LEU	B	33	71.521	-13.207	17.312	1.00	36.34	8
	ATOM	2437	CB	LEU	B	33	68.616	-12.717	16.279	1.00	30.07	6
	ATOM	2438	CG	LEU	B	33	67.670	-12.217	15.191	1.00	29.98	6
30	ATOM	2439	CD1	LEU	B	33	66.434	-13.121	15.083	1.00	31.08	6
	ATOM	2440	CD2	LEU	B	33	67.221	-10.777	15.431	1.00	28.84	6
	ATOM	2441	N	HIS	B	34	70.295	-11.945	18.774	1.00	35.85	7
	ATOM	2442	CA	HIS	B	34	71.004	-12.381	19.965	1.00	39.05	6
	ATOM	2443	C	HIS	B	34	69.976	-12.567	21.067	1.00	37.94	6
35	ATOM	2444	O	HIS	B	34	68.762	-12.451	20.791	1.00	37.26	8
	ATOM	2445	CB	HIS	B	34	72.097	-11.404	20.404	1.00	40.15	6
	ATOM	2446	CG	HIS	B	34	71.668	-10.006	20.714	1.00	42.43	6
	ATOM	2447	ND1	HIS	B	34	70.876	-9.671	21.799	1.00	44.12	7
	ATOM	2448	CD2	HIS	B	34	71.953	-8.848	20.062	1.00	43.13	6
40	ATOM	2449	CE1	HIS	B	34	70.689	-8.360	21.808	1.00	44.28	6
	ATOM	2450	NE2	HIS	B	34	71.323	-7.840	20.763	1.00	44.67	7
	ATOM	2451	N	ASP	B	35	70.439	-12.874	22.263	1.00	36.30	7
	ATOM	2452	CA	ASP	B	35	69.531	-13.176	23.352	1.00	38.71	6
	ATOM	2453	C	ASP	B	35	68.539	-12.055	23.649	1.00	38.11	6
45	ATOM	2454	O	ASP	B	35	67.448	-12.373	24.116	1.00	38.15	8
	ATOM	2455	CB	ASP	B	35	70.309	-13.480	24.637	1.00	43.89	6
	ATOM	2456	CG	ASP	B	35	71.071	-14.776	24.631	1.00	48.19	6
	ATOM	2457	OD1	ASP	B	35	71.046	-15.496	23.603	1.00	50.75	8
	ATOM	2458	OD2	ASP	B	35	71.701	-15.074	25.689	1.00	51.91	8
50	ATOM	2459	N	GLY	B	36	68.919	-10.788	23.499	1.00	35.59	7
	ATOM	2460	CA	GLY	B	36	68.007	-9.688	23.778	1.00	33.96	6
	ATOM	2461	C	GLY	B	36	66.844	-9.774	22.751	1.00	32.11	6
	ATOM	2462	O	GLY	B	36	65.738	-9.524	23.235	1.00	30.98	8
	ATOM	2463	N	HIS	B	37	67.149	-10.177	21.521	1.00	31.48	7
55	ATOM	2464	CA	HIS	B	37	66.006	-10.322	20.581	1.00	31.68	6
	ATOM	2465	C	HIS	B	37	65.118	-11.479	20.969	1.00	33.06	6
	ATOM	2466	O	HIS	B	37	63.861	-11.440	20.850	1.00	30.99	8
	ATOM	2467	CB	HIS	B	37	66.507	-10.514	19.175	1.00	31.96	6
	ATOM	2468	CG	HIS	B	37	67.366	-9.425	18.643	1.00	34.37	6
60	ATOM	2469	ND1	HIS	B	37	66.888	-8.299	18.005	1.00	37.43	7
	ATOM	2470	CD2	HIS	B	37	68.714	-9.330	18.624	1.00	34.96	6
	ATOM	2471	CE1	HIS	B	37	67.890	-7.535	17.580	1.00	35.54	6
	ATOM	2472	NE2	HIS	B	37	69.003	-8.153	17.962	1.00	39.23	7
	ATOM	2473	N	MET	B	38	65.704	-12.577	21.486	1.00	31.32	7
65	ATOM	2474	CA	MET	B	38	64.880	-13.668	22.001	1.00	31.44	6
	ATOM	2475	C	MET	B	38	63.959	-13.252	23.115	1.00	29.66	6
	ATOM	2476	O	MET	B	38	62.851	-13.809	23.253	1.00	28.40	8
	ATOM	2477	CB	MET	B	38	65.799	-14.827	21.487	1.00	34.21	6
	ATOM	2478	CG	MET	B	38	66.423	-15.620	21.375	1.00	35.15	6
70	ATOM	2479	SD	MET	B	38	65.631	-15.970	19.832	1.00	35.12	16
	ATOM	2480	CE	MET	B	38	66.123	-14.628	18.770	1.00	36.33	6
	ATOM	2481	N	LYS	B	39	64.228	-12.300	23.996	1.00	29.09	7
	ATOM	2482	CA	LYS	B	39	63.368	-11.857	25.065	1.00	26.18	6
	ATOM	2483	C	LYS	B	39	62.142	-11.078	24.470	1.00	25.41	6
	ATOM	2484	O	LYS	B	39	61.042	-11.228	24.964	1.00	26.08	8

-70-

	ATOM	2485	CB	LYS	B	39	64.048	-10.935	26.076	1.00	27.75	6
	ATOM	2486	CG	LYS	B	39	63.195	-10.551	27.262	1.00	27.45	6
	ATOM	2487	CD	LYS	B	39	64.031	-9.643	28.216	1.00	30.13	6
5	ATOM	2488	CE	LYS	B	39	63.142	-9.261	29.377	1.00	29.21	6
	ATOM	2489	NZ	LYS	B	39	63.883	-8.413	30.361	1.00	32.36	7
	ATOM	2490	N	LEU	B	40	62.394	-10.379	23.402	1.00	26.07	7
	ATOM	2491	CA	LEU	B	40	61.256	-9.741	22.709	1.00	25.52	6
	ATOM	2492	C	LEU	B	40	60.254	-10.805	22.220	1.00	25.72	6
10	ATOM	2493	O	LEU	B	40	59.055	-10.609	22.293	1.00	23.50	8
	ATOM	2494	CB	LEU	B	40	61.702	-8.954	21.497	1.00	26.47	6
	ATOM	2495	CG	LEU	B	40	62.739	-7.859	21.758	1.00	30.07	6
	ATOM	2496	CD1	LEU	B	40	63.073	-7.128	20.474	1.00	31.00	6
	ATOM	2497	CD2	LEU	B	40	62.237	-6.905	22.832	1.00	30.41	6
15	ATOM	2498	N	VAL	B	41	60.844	-11.842	21.611	1.00	25.04	7
	ATOM	2499	CA	VAL	B	41	59.995	-12.936	21.065	1.00	24.43	6
	ATOM	2500	C	VAL	B	41	59.235	-13.579	22.162	1.00	23.84	6
	ATOM	2501	O	VAL	B	41	58.037	-13.868	22.103	1.00	23.75	8
	ATOM	2502	CB	VAL	B	41	60.893	-13.922	20.289	1.00	24.40	6
20	ATOM	2503	CG1	VAL	B	41	60.057	-15.140	19.914	1.00	24.57	6
	ATOM	2504	CG2	VAL	B	41	61.496	-13.337	19.019	1.00	25.66	6
	ATOM	2505	N	ASP	B	42	59.826	-13.850	23.376	1.00	25.85	7
	ATOM	2506	CA	ASP	B	42	59.130	-14.426	24.480	1.00	26.19	6
	ATOM	2507	C	ASP	B	42	57.994	-13.543	24.981	1.00	28.20	6
25	ATOM	2508	O	ASP	B	42	56.910	-14.030	25.341	1.00	27.55	8
	ATOM	2509	CB	ASP	B	42	60.131	-14.709	25.659	1.00	29.50	6
	ATOM	2510	CG	ASP	B	42	61.118	-15.822	25.377	1.00	32.71	6
	ATOM	2511	OD1	ASP	B	42	61.051	-16.616	24.419	1.00	33.03	8
	ATOM	2512	OD2	ASP	B	42	62.135	-15.893	26.160	1.00	33.67	8
30	ATOM	2513	N	GLU	B	43	58.205	-12.216	24.957	1.00	26.23	7
	ATOM	2514	CA	GLU	B	43	57.130	-11.321	25.355	1.00	27.21	6
	ATOM	2515	C	GLU	B	43	55.973	-11.339	24.327	1.00	24.30	6
	ATOM	2516	O	GLU	B	43	54.809	-11.340	24.709	1.00	24.66	8
	ATOM	2517	CB	GLU	B	43	57.676	-9.912	25.475	1.00	30.67	6
35	ATOM	2518	CG	GLU	B	43	56.740	-8.904	26.130	1.00	36.81	6
	ATOM	2519	CD	GLU	B	43	56.445	-9.257	27.585	1.00	40.25	6
	ATOM	2520	OE1	GLU	B	43	57.347	-9.847	28.236	1.00	44.07	8
	ATOM	2521	OE2	GLU	B	43	55.348	-8.999	28.121	1.00	40.92	8
	ATOM	2522	N	ALA	B	44	56.324	-11.466	23.083	1.00	26.35	7
40	ATOM	2523	CA	ALA	B	44	55.321	-11.474	21.969	1.00	23.41	6
	ATOM	2524	C	ALA	B	44	54.526	-12.754	22.079	1.00	26.63	6
	ATOM	2525	O	ALA	B	44	53.287	-12.728	22.074	1.00	26.61	8
	ATOM	2526	CB	ALA	B	44	56.007	-11.299	20.651	1.00	25.41	6
	ATOM	2527	N	LYS	B	45	55.209	-13.882	22.329	1.00	27.34	7
45	ATOM	2528	CA	LYS	B	45	54.542	-15.169	22.501	1.00	29.71	6
	ATOM	2529	C	LYS	B	45	53.589	-15.160	23.659	1.00	28.45	6
	ATOM	2530	O	LYS	B	45	52.559	-15.805	23.717	1.00	28.18	8
	ATOM	2531	CB	LYS	B	45	55.537	-16.322	22.783	1.00	32.90	6
	ATOM	2532	CG	LYS	B	45	56.368	-16.726	21.588	1.00	38.80	6
50	ATOM	2533	CD	LYS	B	45	57.724	-17.301	21.961	1.00	43.49	6
	ATOM	2534	CE	LYS	B	45	57.757	-18.398	23.004	1.00	46.00	6
	ATOM	2535	NZ	LYS	B	45	59.077	-18.396	23.727	1.00	47.62	7
	ATOM	2536	N	ALA	B	46	53.935	-14.446	24.748	1.00	27.58	7
	ATOM	2537	CA	ALA	B	46	53.076	-14.389	25.900	1.00	27.60	6
55	ATOM	2538	C	ALA	B	46	51.831	-13.527	25.751	1.00	28.91	6
	ATOM	2539	O	ALA	B	46	50.905	-13.633	26.549	1.00	30.19	8
	ATOM	2540	CB	ALA	B	46	53.882	-13.818	27.097	1.00	28.29	6
	ATOM	2541	N	ARG	B	47	51.754	-12.657	24.741	1.00	26.88	7
	ATOM	2542	CA	ARG	B	47	50.691	-11.719	24.586	1.00	25.76	6
60	ATOM	2543	C	ARG	B	47	49.781	-11.972	23.373	1.00	23.01	6
	ATOM	2544	O	ARG	B	47	48.813	-11.243	23.291	1.00	23.89	8
	ATOM	2545	CB	ARG	B	47	51.345	-10.312	24.433	1.00	24.92	6
	ATOM	2546	CG	ARG	B	47	51.975	-9.858	25.800	1.00	27.22	6
	ATOM	2547	CD	ARG	B	47	52.755	-8.575	25.491	1.00	29.69	6
65	ATOM	2548	NE	ARG	B	47	53.415	-7.966	26.670	1.00	34.33	7
	ATOM	2549	CZ	ARG	B	47	52.861	-6.966	27.358	1.00	35.85	6
	ATOM	2550	NH1	ARG	B	47	51.680	-6.442	27.073	1.00	35.22	7
	ATOM	2551	NH2	ARG	B	47	53.555	-6.467	28.392	1.00	37.54	7
	ATOM	2552	N	ALA	B	48	50.203	-12.899	22.529	1.00	23.33	7
70	ATOM	2553	CA	ALA	B	48	49.413	-13.114	21.284	1.00	23.32	6
	ATOM	2554	C	ALA	B	48	49.405	-14.574	20.933	1.00	26.45	6
	ATOM	2555	O	ALA	B	48	50.224	-15.356	21.466	1.00	24.59	8
	ATOM	2556	CB	ALA	B	48	50.059	-12.332	20.168	1.00	23.24	6
	ATOM	2557	N	ASP	B	49	48.547	-15.010	20.004	1.00	24.54	7
	ATOM	2558	CA	ASP	B	49	48.537	-16.394	19.594	1.00	24.90	6

-71-

	ATOM	2559	C	ASP	B	49	49.677	-16.770	18.689	1.00	24.42	6
	ATOM	2560	O	ASP	B	49	50.254	-17.869	18.668	1.00	26.07	8
	ATOM	2561	CB	ASP	B	49	47.237	-16.656	18.803	1.00	26.28	6
5	ATOM	2562	CG	ASP	B	49	45.979	-16.417	19.627	1.00	30.04	6
	ATOM	2563	OD1	ASP	B	49	45.977	-16.990	20.754	1.00	32.57	8
	ATOM	2564	OD2	ASP	B	49	45.038	-15.712	19.183	1.00	30.75	8
	ATOM	2565	N	VAL	B	50	50.004	-15.842	17.792	1.00	20.95	7
	ATOM	2566	CA	VAL	B	50	50.980	-15.998	16.747	1.00	20.87	6
10	ATOM	2567	C	VAL	B	50	52.014	-14.905	16.734	1.00	20.83	6
	ATOM	2568	O	VAL	B	50	51.742	-13.704	16.973	1.00	20.70	8
	ATOM	2569	CB	VAL	B	50	50.241	-16.031	15.369	1.00	22.53	6
	ATOM	2570	CG1	VAL	B	50	51.112	-15.780	14.170	1.00	26.09	6
	ATOM	2571	CG2	VAL	B	50	49.536	-17.393	15.199	1.00	25.40	6
15	ATOM	2572	N	VAL	B	51	53.286	-15.325	16.567	1.00	19.42	7
	ATOM	2573	CA	VAL	B	51	54.373	-14.336	16.498	1.00	22.20	6
	ATOM	2574	C	VAL	B	51	54.975	-14.279	15.113	1.00	22.35	6
	ATOM	2575	O	VAL	B	51	55.400	-15.274	14.488	1.00	23.37	8
	ATOM	2576	CB	VAL	B	51	55.498	-14.618	17.516	1.00	23.80	6
20	ATOM	2577	CG1	VAL	B	51	56.616	-13.574	17.449	1.00	24.48	6
	ATOM	2578	CG2	VAL	B	51	54.855	-14.682	18.910	1.00	28.00	6
	ATOM	2579	N	VAL	B	52	55.108	-13.080	14.590	1.00	18.68	7
	ATOM	2580	CA	VAL	B	52	55.734	-12.772	13.322	1.00	17.55	6
	ATOM	2581	C	VAL	B	52	57.014	-11.980	13.623	1.00	21.15	6
25	ATOM	2582	O	VAL	B	52	56.930	-10.957	14.319	1.00	19.41	8
	ATOM	2583	CB	VAL	B	52	54.885	-11.936	12.341	1.00	19.87	6
	ATOM	2584	CG1	VAL	B	52	55.613	-11.467	11.107	1.00	19.90	6
	ATOM	2585	CG2	VAL	B	52	53.651	-12.759	11.943	1.00	20.31	6
	ATOM	2586	N	VAL	B	53	58.150	-12.469	13.104	1.00	20.72	7
30	ATOM	2587	CA	VAL	B	53	59.396	-11.698	13.267	1.00	20.35	6
	ATOM	2588	C	VAL	B	53	59.854	-11.261	11.925	1.00	22.26	6
	ATOM	2589	O	VAL	B	53	59.933	-12.026	10.948	1.00	23.47	8
	ATOM	2590	CB	VAL	B	53	60.505	-12.545	13.977	1.00	20.44	6
	ATOM	2591	CG1	VAL	B	53	61.791	-11.700	14.053	1.00	22.35	6
35	ATOM	2592	CG2	VAL	B	53	60.059	-13.004	15.346	1.00	22.26	6
	ATOM	2593	N	SER	B	54	60.144	-9.957	11.694	1.00	20.14	7
	ATOM	2594	CA	SER	B	54	60.629	-9.453	10.425	1.00	20.53	6
	ATOM	2595	C	SER	B	54	62.157	-9.208	10.601	1.00	23.03	6
	ATOM	2596	O	SER	B	54	62.594	-8.867	11.697	1.00	23.22	8
40	ATOM	2597	CB	SER	B	54	59.973	-8.182	9.883	1.00	24.56	6
	ATOM	2598	OG	SER	B	54	60.079	-7.161	10.861	1.00	24.52	8
	ATOM	2599	N	ILE	B	55	62.804	-9.615	9.537	1.00	25.11	7
	ATOM	2600	CA	ILE	B	55	64.289	-9.443	9.508	1.00	23.93	6
	ATOM	2601	C	ILE	B	55	64.589	-8.756	8.220	1.00	22.42	6
45	ATOM	2602	O	ILE	B	55	64.333	-9.214	7.082	1.00	23.75	8
	ATOM	2603	CB	ILE	B	55	65.017	-10.788	9.599	1.00	25.95	6
	ATOM	2604	CG1	ILE	B	55	64.888	-11.494	10.920	1.00	25.74	6
	ATOM	2605	CG2	ILE	B	55	66.512	-10.480	9.307	1.00	26.43	6
	ATOM	2606	CD1	ILE	B	55	65.315	-12.955	10.805	1.00	29.38	6
50	ATOM	2607	N	PHE	B	56	65.039	-7.469	8.273	1.00	23.02	7
	ATOM	2608	CA	PHE	B	56	65.225	-6.624	7.153	1.00	24.66	6
	ATOM	2609	C	PHE	B	56	66.202	-5.465	7.454	1.00	26.79	6
	ATOM	2610	O	PHE	B	56	65.937	-4.712	8.392	1.00	26.50	8
	ATOM	2611	CB	PHE	B	56	63.878	-6.011	6.668	1.00	22.93	6
55	ATOM	2612	CG	PHE	B	56	64.081	-5.130	5.476	1.00	24.37	6
	ATOM	2613	CD1	PHE	B	56	64.570	-5.602	4.262	1.00	25.67	6
	ATOM	2614	CD2	PHE	B	56	63.711	-3.781	5.549	1.00	23.80	6
	ATOM	2615	CE1	PHE	B	56	64.765	-4.758	3.193	1.00	25.30	6
	ATOM	2616	CE2	PHE	B	56	63.882	-2.969	4.441	1.00	25.84	6
60	ATOM	2617	CZ	PHE	B	56	64.399	-3.429	3.249	1.00	27.27	6
	ATOM	2618	N	VAL	B	57	67.330	-5.512	6.717	1.00	28.13	7
	ATOM	2619	CA	VAL	B	57	68.347	-4.471	7.001	1.00	27.59	6
	ATOM	2620	C	VAL	B	57	67.968	-3.357	6.089	1.00	26.50	6
	ATOM	2621	O	VAL	B	57	68.047	-3.404	4.871	1.00	28.47	8
65	ATOM	2622	CB	VAL	B	57	69.787	-5.034	6.846	1.00	28.54	6
	ATOM	2623	CG1	VAL	B	57	70.795	-3.915	7.235	1.00	30.14	6
	ATOM	2624	CG2	VAL	B	57	70.028	-6.232	7.674	1.00	27.80	6
	ATOM	2625	N	ASN	B	58	67.280	-2.367	6.723	1.00	27.33	7
	ATOM	2626	CA	ASN	B	58	66.643	-1.277	5.989	1.00	28.47	6
70	ATOM	2627	C	ASN	B	58	67.589	-0.208	5.529	1.00	28.30	6
	ATOM	2628	O	ASN	B	58	68.068	0.587	6.350	1.00	29.87	8
	ATOM	2629	CB	ASN	B	58	65.608	-0.711	7.004	1.00	27.68	6
	ATOM	2630	CG	ASN	B	58	64.919	0.542	6.507	1.00	24.26	6
	ATOM	2631	OD1	ASN	B	58	64.739	0.717	5.301	1.00	26.55	8
	ATOM	2632	ND2	ASN	B	58	64.487	1.392	7.445	1.00	24.78	7

-72-

	ATOM	2633	N	PRO	B	59	67.828	-0.063	4.251	1.00	32.20	7
	ATOM	2634	CA	PRO	B	59	68.766	0.929	3.749	1.00	32.85	6
	ATOM	2635	C	PRO	B	59	68.415	2.336	4.177	1.00	35.54	6
5	ATOM	2636	O	PRO	B	59	69.298	3.191	4.360	1.00	33.70	8
	ATOM	2637	CB	PRO	B	59	68.703	0.729	2.239	1.00	36.08	6
	ATOM	2638	CG	PRO	B	59	68.404	-0.761	2.113	1.00	35.06	6
	ATOM	2639	CD	PRO	B	59	67.336	-0.957	3.170	1.00	34.20	6
	ATOM	2640	N	MET	B	60	67.111	2.642	4.360	1.00	34.39	7
10	ATOM	2641	CA	MET	B	60	66.683	3.994	4.699	1.00	36.32	6
	ATOM	2642	C	MET	B	60	67.197	4.523	6.022	1.00	37.35	6
	ATOM	2643	O	MET	B	60	67.169	5.772	6.239	1.00	38.05	8
	ATOM	2644	CB	MET	B	60	65.148	4.088	4.790	1.00	37.91	6
	ATOM	2645	CG	MET	B	60	64.450	4.720	3.624	1.00	39.92	6
15	ATOM	2646	SD	MET	B	60	62.934	5.666	4.060	1.00	39.02	16
	ATOM	2647	CE	MET	B	60	61.890	5.076	2.719	1.00	40.24	6
	ATOM	2648	N	GLN	B	61	67.520	3.632	6.950	1.00	36.15	7
	ATOM	2649	CA	GLN	B	61	67.973	4.079	8.262	1.00	37.72	6
	ATOM	2650	C	GLN	B	61	69.493	3.884	8.375	1.00	39.87	6
20	ATOM	2651	O	GLN	B	61	70.042	3.727	9.476	1.00	42.79	8
	ATOM	2652	CB	GLN	B	61	67.179	3.390	9.361	1.00	35.80	6
	ATOM	2653	CG	GLN	B	61	67.540	1.949	9.681	1.00	32.41	6
	ATOM	2654	CD	GLN	B	61	66.514	1.303	10.572	1.00	29.81	6
	ATOM	2655	OE1	GLN	B	61	65.349	0.972	10.194	1.00	28.50	8
25	ATOM	2656	NE2	GLN	B	61	66.860	0.939	11.787	1.00	27.42	7
	ATOM	2657	N	PHE	B	62	70.210	3.961	7.244	1.00	39.42	7
	ATOM	2658	CA	PHE	B	62	71.665	3.901	7.241	1.00	40.52	6
	ATOM	2659	C	PHE	B	62	72.216	5.205	6.643	1.00	43.48	6
	ATOM	2660	O	PHE	B	62	71.742	5.679	5.613	1.00	41.80	8
30	ATOM	2661	CB	PHE	B	62	72.285	2.727	6.462	1.00	39.44	6
	ATOM	2662	CG	PHE	B	62	72.261	1.476	7.310	1.00	38.25	6
	ATOM	2663	CD1	PHE	B	62	71.094	0.697	7.350	1.00	37.73	6
	ATOM	2664	CD2	PHE	B	62	73.329	1.085	8.076	1.00	37.32	6
	ATOM	2665	CE1	PHE	B	62	71.053	-0.422	8.157	1.00	37.14	6
35	ATOM	2666	CE2	PHE	B	62	73.294	-0.044	8.870	1.00	36.89	6
	ATOM	2667	CZ	PHE	B	62	72.145	-0.825	8.902	1.00	37.49	6
	ATOM	2668	N	ASP	B	63	73.267	5.723	7.257	1.00	48.37	7
	ATOM	2669	CA	ASP	B	63	73.887	6.980	6.816	1.00	51.97	6
	ATOM	2670	C	ASP	B	63	74.709	6.872	5.539	1.00	53.02	6
40	ATOM	2671	O	ASP	B	63	74.642	7.765	4.679	1.00	53.58	8
	ATOM	2672	CB	ASP	B	63	74.800	7.511	7.922	1.00	53.54	6
	ATOM	2673	CG	ASP	B	63	74.087	7.668	9.251	1.00	55.47	6
	ATOM	2674	OD1	ASP	B	63	72.832	7.712	9.265	1.00	57.99	8
	ATOM	2675	OD2	ASP	B	63	74.767	7.751	10.294	1.00	56.33	8
45	ATOM	2676	N	ARG	B	64	75.521	5.830	5.420	1.00	52.77	7
	ATOM	2677	CA	ARG	B	64	76.344	5.697	4.211	1.00	54.08	6
	ATOM	2678	C	ARG	B	64	76.323	4.250	3.759	1.00	54.41	6
	ATOM	2679	O	ARG	B	64	76.037	3.392	4.582	1.00	53.32	8
	ATOM	2680	CB	ARG	B	64	77.758	6.205	4.486	1.00	53.78	6
50	ATOM	2681	N	PRO	B	65	76.658	3.987	2.505	1.00	56.79	7
	ATOM	2682	CA	PRO	B	65	76.654	2.637	1.974	1.00	57.90	6
	ATOM	2683	C	PRO	B	65	77.533	1.632	2.682	1.00	59.54	6
	ATOM	2684	O	PRO	B	65	77.159	0.456	2.659	1.00	59.29	8
	ATOM	2685	CB	PRO	B	65	77.123	2.790	0.528	1.00	58.01	6
55	ATOM	2686	CG	PRO	B	65	77.017	4.235	0.201	1.00	58.02	6
	ATOM	2687	CD	PRO	B	65	77.011	5.007	1.489	1.00	57.36	6
	ATOM	2688	N	GLU	B	66	78.651	1.990	3.291	1.00	60.73	7
	ATOM	2689	CA	GLU	B	66	79.545	1.029	3.926	1.00	60.74	6
	ATOM	2690	C	GLU	B	66	78.996	0.590	5.268	1.00	58.41	6
60	ATOM	2691	O	GLU	B	66	79.184	-0.554	5.672	1.00	59.32	8
	ATOM	2692	CB	GLU	B	66	80.949	1.612	4.114	1.00	63.95	6
	ATOM	2693	CG	GLU	B	66	81.554	2.085	2.807	1.00	67.09	6
	ATOM	2694	CD	GLU	B	66	81.129	3.469	2.387	1.00	69.60	6
	ATOM	2695	OE1	GLU	B	66	80.077	4.027	2.774	1.00	71.11	8
65	ATOM	2696	OE2	GLU	B	66	81.873	4.122	1.612	1.00	71.37	8
	ATOM	2697	N	ASP	B	67	78.271	1.521	5.890	1.00	55.22	7
	ATOM	2698	CA	ASP	B	67	77.618	1.142	7.151	1.00	53.44	6
	ATOM	2699	C	ASP	B	67	76.586	0.068	6.773	1.00	49.67	6
	ATOM	2700	O	ASP	B	67	76.505	-0.978	7.418	1.00	47.57	8
70	ATOM	2701	CB	ASP	B	67	77.109	2.400	7.818	1.00	55.45	6
	ATOM	2702	CG	ASP	B	67	78.226	3.389	8.134	1.00	58.05	6
	ATOM	2703	OD1	ASP	B	67	79.352	3.283	7.602	1.00	58.16	8
	ATOM	2704	OD2	ASP	B	67	77.993	4.307	8.954	1.00	58.74	8
	ATOM	2705	N	LEU	B	68	75.906	0.243	5.640	1.00	47.47	7
	ATOM	2706	CA	LEU	B	68	74.908	-0.706	5.170	1.00	45.94	6

-73-

	ATOM	2707	C	LEU	B	68	75.575	-2.002	4.715	1.00	46.59	6
	ATOM	2708	O	LEU	B	68	75.241	-3.082	5.201	1.00	47.70	8
	ATOM	2709	CB	LEU	B	68	74.066	-0.198	4.001	1.00	44.25	6
	ATOM	2710	CG	LEU	B	68	72.989	-1.184	3.489	1.00	42.50	6
5	ATOM	2711	CD1	LEU	B	68	72.064	-1.563	4.634	1.00	40.69	6
	ATOM	2712	CD2	LEU	B	68	72.214	-0.620	2.317	1.00	42.43	6
	ATOM	2713	N	ALA	B	69	76.513	-1.866	3.793	1.00	46.99	7
	ATOM	2714	CA	ALA	B	69	77.238	-3.024	3.259	1.00	47.49	6
10	ATOM	2715	C	ALA	B	69	77.930	-3.829	4.337	1.00	46.64	6
	ATOM	2716	O	ALA	B	69	77.913	-5.072	4.256	1.00	48.02	8
	ATOM	2717	CB	ALA	B	69	78.258	-2.532	2.235	1.00	48.47	6
	ATOM	2718	N	ARG	B	70	78.475	-3.201	5.370	1.00	45.74	7
	ATOM	2719	CA	ARG	B	70	79.158	-3.961	6.411	1.00	44.24	6
15	ATOM	2720	C	ARG	B	70	78.246	-4.487	7.495	1.00	44.00	6
	ATOM	2721	O	ARG	B	70	78.700	-5.308	8.281	1.00	41.15	8
	ATOM	2722	CB	ARG	B	70	80.247	-3.071	7.038	1.00	46.62	6
	ATOM	2723	N	TYR	B	71	76.966	-4.108	7.573	1.00	41.84	7
	ATOM	2724	CA	TYR	B	71	76.076	-4.624	8.609	1.00	39.35	6
20	ATOM	2725	C	TYR	B	71	75.935	-6.141	8.508	1.00	37.54	6
	ATOM	2726	O	TYR	B	71	75.788	-6.673	7.410	1.00	37.39	8
	ATOM	2727	CB	TYR	B	71	74.712	-3.919	8.487	1.00	38.73	6
	ATOM	2728	CG	TYR	B	71	73.927	-4.054	9.778	1.00	36.95	6
	ATOM	2729	CD1	TYR	B	71	74.099	-3.155	10.806	1.00	34.97	6
25	ATOM	2730	CD2	TYR	B	71	72.993	-5.079	9.946	1.00	35.71	6
	ATOM	2731	CE1	TYR	B	71	73.405	-3.260	12.004	1.00	35.01	6
	ATOM	2732	CE2	TYR	B	71	72.287	-5.192	11.109	1.00	33.37	6
	ATOM	2733	CZ	TYR	B	71	72.462	-4.292	12.119	1.00	34.69	6
	ATOM	2734	OH	TYR	B	71	71.765	-4.407	13.290	1.00	34.77	8
30	ATOM	2735	N	PRO	B	72	75.985	-6.835	9.625	1.00	37.73	7
	ATOM	2736	CA	PRO	B	72	76.030	-8.293	9.644	1.00	40.09	6
	ATOM	2737	C	PRO	B	72	74.756	-8.966	9.194	1.00	42.74	6
	ATOM	2738	O	PRO	B	72	73.697	-8.753	9.783	1.00	42.94	8
	ATOM	2739	CB	PRO	B	72	76.369	-8.681	11.080	1.00	39.27	6
35	ATOM	2740	CG	PRO	B	72	76.366	-7.442	11.876	1.00	39.73	6
	ATOM	2741	CD	PRO	B	72	76.222	-6.266	10.967	1.00	37.89	6
	ATOM	2742	N	ARG	B	73	74.856	-9.773	8.147	1.00	42.53	7
	ATOM	2743	CA	ARG	B	73	73.687	-10.492	7.639	1.00	43.36	6
	ATOM	2744	C	ARG	B	73	73.881	-11.945	7.992	1.00	43.07	6
40	ATOM	2745	O	ARG	B	73	74.875	-12.526	7.534	1.00	42.68	8
	ATOM	2746	CB	ARG	B	73	73.524	-10.225	6.143	1.00	45.53	6
	ATOM	2747	CG	ARG	B	73	73.306	-8.700	5.962	1.00	48.13	6
	ATOM	2748	CD	ARG	B	73	72.868	-8.393	4.559	1.00	49.65	6
	ATOM	2749	NE	ARG	B	73	72.537	-7.021	4.268	1.00	51.16	7
45	ATOM	2750	CZ	ARG	B	73	73.255	-5.930	4.486	1.00	51.88	6
	ATOM	2751	NH1	ARG	B	73	74.449	-5.968	5.071	1.00	53.24	7
	ATOM	2752	NH2	ARG	B	73	72.779	-4.755	4.085	1.00	51.96	7
	ATOM	2753	N	THR	B	74	73.054	-12.505	8.869	1.00	40.78	7
	ATOM	2754	CA	THR	B	74	73.184	-13.870	9.338	1.00	38.76	6
50	ATOM	2755	C	THR	B	74	71.806	-14.564	9.373	1.00	36.02	6
	ATOM	2756	O	THR	B	74	71.381	-15.074	10.395	1.00	35.74	8
	ATOM	2757	CB	THR	B	74	73.825	-13.949	10.726	1.00	39.81	6
	ATOM	2758	OG1	THR	B	74	72.965	-13.304	11.686	1.00	41.92	8
	ATOM	2759	CG2	THR	B	74	75.176	-13.231	10.872	1.00	39.68	6
55	ATOM	2760	N	LEU	B	75	71.163	-14.648	8.241	1.00	38.12	7
	ATOM	2761	CA	LEU	B	75	69.795	-15.148	8.140	1.00	38.95	6
	ATOM	2762	C	LEU	B	75	69.657	-16.574	8.644	1.00	39.45	6
	ATOM	2763	O	LEU	B	75	68.791	-16.843	9.478	1.00	37.24	8
	ATOM	2764	CB	LEU	B	75	69.269	-15.024	6.693	1.00	41.95	6
60	ATOM	2765	CG	LEU	B	75	67.785	-15.355	6.505	1.00	42.42	6
	ATOM	2766	CD1	LEU	B	75	66.907	-14.527	7.453	1.00	43.76	6
	ATOM	2767	CD2	LEU	B	75	67.332	-15.146	5.070	1.00	42.41	6
	ATOM	2768	N	GLN	B	76	70.525	-17.509	8.187	1.00	39.28	7
	ATOM	2769	CA	GLN	B	76	70.400	-18.884	8.667	1.00	39.73	6
65	ATOM	2770	C	GLN	B	76	70.476	-18.965	10.181	1.00	36.54	6
	ATOM	2771	O	GLN	B	76	69.671	-19.700	10.759	1.00	35.73	8
	ATOM	2772	CB	GLN	B	76	71.477	-19.872	8.150	1.00	42.75	6
	ATOM	2773	CG	GLN	B	76	71.375	-21.209	8.897	1.00	45.19	6
	ATOM	2774	CD	GLN	B	76	72.464	-22.227	8.683	1.00	48.00	6
70	ATOM	2775	OE1	GLN	B	76	72.386	-23.355	9.236	1.00	51.20	8
	ATOM	2776	NE2	GLN	B	76	73.482	-21.896	7.921	1.00	46.67	7
	ATOM	2777	N	GLU	B	77	71.442	-18.317	10.808	1.00	33.90	7
	ATOM	2778	CA	GLU	B	77	71.585	-18.356	12.259	1.00	33.25	6
	ATOM	2779	C	GLU	B	77	70.408	-17.708	13.013	1.00	32.48	6
	ATOM	2780	O	GLU	B	77	69.960	-18.170	14.072	1.00	31.46	8

-74-

	ATOM	2781	CB	GLU	B	77	72.885	-17.636	12.627	1.00	33.79	6
	ATOM	2782	N	ASP	B	78	69.915	-16.625	12.388	1.00	32.55	7
	ATOM	2783	CA	ASP	B	78	68.738	-15.937	12.973	1.00	30.24	6
5	ATOM	2784	C	ASP	B	78	67.576	-16.964	12.993	1.00	28.55	6
	ATOM	2785	O	ASP	B	78	66.981	-17.174	14.032	1.00	29.32	8
	ATOM	2786	CB	ASP	B	78	68.337	-14.697	12.209	1.00	31.08	6
	ATOM	2787	CG	ASP	B	78	69.331	-13.551	12.195	1.00	34.64	6
	ATOM	2788	OD1	ASP	B	78	70.144	-13.494	13.151	1.00	37.80	8
10	ATOM	2789	OD2	ASP	B	78	69.328	-12.744	11.228	1.00	36.82	8
	ATOM	2790	N	CYS	B	79	67.355	-17.543	11.825	1.00	30.19	7
	ATOM	2791	CA	CYS	B	79	66.231	-18.500	11.625	1.00	33.57	6
	ATOM	2792	C	CYS	B	79	66.327	-19.720	12.495	1.00	35.51	6
	ATOM	2793	O	CYS	B	79	65.350	-20.136	13.149	1.00	34.66	8
15	ATOM	2794	CB	CYS	B	79	66.184	-18.792	10.132	1.00	33.80	6
	ATOM	2795	SG	CYS	B	79	65.381	-17.456	9.190	1.00	37.92	16
	ATOM	2796	N	GLU	B	80	67.543	-20.281	12.707	1.00	36.68	7
	ATOM	2797	CA	GLU	B	80	67.692	-21.347	13.691	1.00	35.97	6
	ATOM	2798	C	GLU	B	80	67.370	-20.883	15.088	1.00	33.68	6
	ATOM	2799	O	GLU	B	80	66.764	-21.625	15.883	1.00	34.88	8
20	ATOM	2800	CB	GLU	B	80	69.130	-21.906	13.660	1.00	36.66	6
	ATOM	2801	N	LYS	B	81	67.668	-19.638	15.520	1.00	34.02	7
	ATOM	2802	CA	LYS	B	81	67.277	-19.253	16.875	1.00	31.36	6
	ATOM	2803	C	LYS	B	81	65.756	-19.047	17.017	1.00	30.38	6
25	ATOM	2804	O	LYS	B	81	65.183	-19.326	18.068	1.00	29.64	8
	ATOM	2805	CB	LYS	B	81	67.967	-17.965	17.314	1.00	35.26	6
	ATOM	2806	CG	LYS	B	81	69.451	-18.114	17.566	1.00	37.30	6
	ATOM	2807	CD	LYS	B	81	70.118	-16.744	17.730	1.00	39.14	6
	ATOM	2808	CE	LYS	B	81	71.635	-17.011	17.782	1.00	41.26	6
30	ATOM	2809	NZ	LYS	B	81	72.310	-15.733	18.142	1.00	43.00	7
	ATOM	2810	N	LEU	B	82	65.158	-18.495	15.965	1.00	30.34	7
	ATOM	2811	CA	LEU	B	82	63.700	-18.248	16.019	1.00	30.06	6
	ATOM	2812	C	LEU	B	82	62.914	-19.540	16.028	1.00	32.53	6
	ATOM	2813	O	LEU	B	82	61.880	-19.695	16.694	1.00	32.69	8
35	ATOM	2814	CB	LEU	B	82	63.335	-17.328	14.845	1.00	30.48	6
	ATOM	2815	CG	LEU	B	82	63.981	-15.924	14.936	1.00	28.69	6
	ATOM	2816	CD1	LEU	B	82	63.820	-15.222	13.603	1.00	25.14	6
	ATOM	2817	CD2	LEU	B	82	63.412	-15.105	16.103	1.00	28.77	6
	ATOM	2818	N	ASN	B	83	63.438	-20.549	15.323	1.00	33.22	7
40	ATOM	2819	CA	ASN	B	83	62.748	-21.849	15.282	1.00	36.28	6
	ATOM	2820	C	ASN	B	83	62.747	-22.507	16.648	1.00	36.28	6
	ATOM	2821	O	ASN	B	83	61.735	-23.043	17.139	1.00	35.49	8
	ATOM	2822	CB	ASN	B	83	63.419	-22.656	14.181	1.00	39.05	6
	ATOM	2823	CG	ASN	B	83	62.717	-23.983	13.943	1.00	42.41	6
45	ATOM	2824	OD1	ASN	B	83	63.382	-25.000	14.194	1.00	45.42	8
	ATOM	2825	ND2	ASN	B	83	61.474	-23.962	13.533	1.00	41.68	7
	ATOM	2826	N	LYS	B	84	63.820	-22.351	17.437	1.00	37.37	7
	ATOM	2827	CA	LYS	B	84	63.850	-22.927	18.780	1.00	39.89	6
	ATOM	2828	C	LYS	B	84	62.942	-22.200	19.747	1.00	40.11	6
50	ATOM	2829	O	LYS	B	84	62.533	-22.693	20.801	1.00	40.80	8
	ATOM	2830	CB	LYS	B	84	65.305	-22.932	19.291	1.00	39.81	6
	ATOM	2831	N	ARG	B	85	62.590	-20.942	19.425	1.00	40.09	7
	ATOM	2832	CA	ARG	B	85	61.718	-20.125	20.235	1.00	39.63	6
	ATOM	2833	C	ARG	B	85	60.260	-20.305	19.812	1.00	40.59	6
55	ATOM	2834	O	ARG	B	85	59.373	-19.647	20.334	1.00	42.54	8
	ATOM	2835	CB	ARG	B	85	62.093	-18.647	20.134	1.00	40.48	6
	ATOM	2836	CG	ARG	B	85	62.052	-17.972	21.510	1.00	41.38	6
	ATOM	2837	CD	ARG	B	85	63.336	-18.317	22.253	1.00	42.99	6
	ATOM	2838	NE	ARG	B	85	63.380	-17.724	23.588	1.00	42.49	7
60	ATOM	2839	CZ	ARG	B	85	64.475	-17.764	24.342	1.00	43.47	6
	ATOM	2840	NH1	ARG	B	85	64.483	-17.233	25.553	1.00	42.44	7
	ATOM	2841	NH2	ARG	B	85	65.570	-18.361	23.872	1.00	44.83	7
	ATOM	2842	N	LYS	B	86	60.041	-21.151	18.827	1.00	39.06	7
	ATOM	2843	CA	LYS	B	86	58.702	-21.492	18.348	1.00	38.48	6
65	ATOM	2844	C	LYS	B	86	57.996	-20.296	17.712	1.00	36.35	6
	ATOM	2845	O	LYS	B	86	56.785	-20.127	17.808	1.00	34.81	8
	ATOM	2846	CB	LYS	B	86	57.903	-22.087	19.511	1.00	39.68	6
	ATOM	2847	N	VAL	B	87	58.751	-19.515	16.953	1.00	33.22	7
	ATOM	2848	CA	VAL	B	87	58.133	-18.416	16.204	1.00	29.42	6
70	ATOM	2849	C	VAL	B	87	57.340	-18.986	15.051	1.00	30.11	6
	ATOM	2850	O	VAL	B	87	57.704	-19.959	14.359	1.00	29.33	8
	ATOM	2851	CB	VAL	B	87	59.267	-17.508	15.732	1.00	27.19	6
	ATOM	2852	CG1	VAL	B	87	58.859	-16.637	14.581	1.00	28.11	6
	ATOM	2853	CG2	VAL	B	87	59.756	-16.644	16.909	1.00	28.45	6
	ATOM	2854	N	ASP	B	88	56.179	-18.408	14.740	1.00	27.32	7

-75-

	ATOM	2855	CA	ASP	B	88	55.356	-18.963	13.667	1.00	26.78	6
	ATOM	2856	C	ASP	B	88	55.780	-18.589	12.285	1.00	26.80	6
	ATOM	2857	O	ASP	B	88	55.687	-19.415	11.342	1.00	26.44	8
5	ATOM	2858	CB	ASP	B	88	53.895	-18.488	13.889	1.00	29.04	6
	ATOM	2859	CG	ASP	B	88	53.482	-18.856	15.298	1.00	30.71	6
	ATOM	2860	OD1	ASP	B	88	52.991	-20.020	15.427	1.00	32.60	8
	ATOM	2861	OD2	ASP	B	88	53.717	-18.147	16.323	1.00	30.59	8
	ATOM	2862	N	LEU	B	89	56.204	-17.356	12.062	1.00	23.49	7
10	ATOM	2863	CA	LEU	B	89	56.498	-16.854	10.756	1.00	23.51	6
	ATOM	2864	C	LEU	B	89	57.676	-15.880	10.729	1.00	23.91	6
	ATOM	2865	O	LEU	B	89	57.609	-14.975	11.552	1.00	24.58	8
	ATOM	2866	CB	LEU	B	89	55.236	-16.101	10.292	1.00	26.12	6
	ATOM	2867	CG	LEU	B	89	55.179	-15.845	8.823	1.00	29.47	6
15	ATOM	2868	CD1	LEU	B	89	53.725	-15.783	8.333	1.00	31.30	6
	ATOM	2869	CD2	LEU	B	89	55.883	-14.542	8.494	1.00	32.84	6
	ATOM	2870	N	VAL	B	90	58.629	-15.971	9.842	1.00	23.43	7
	ATOM	2871	CA	VAL	B	90	59.716	-15.006	9.714	1.00	23.35	6
	ATOM	2872	C	VAL	B	90	59.553	-14.315	8.413	1.00	24.66	6
20	ATOM	2873	O	VAL	B	90	59.386	-14.905	7.324	1.00	24.98	8
	ATOM	2874	CB	VAL	B	90	61.116	-15.722	9.862	1.00	23.84	6
	ATOM	2875	CG1	VAL	B	90	62.212	-14.701	9.640	1.00	26.41	6
	ATOM	2876	CG2	VAL	B	90	61.195	-16.379	11.217	1.00	23.75	6
	ATOM	2877	N	PHE	B	91	59.462	-12.972	8.351	1.00	23.00	7
25	ATOM	2878	CA	PHE	B	91	59.363	-12.240	7.147	1.00	21.82	6
	ATOM	2879	C	PHE	B	91	60.754	-11.693	6.787	1.00	24.30	6
	ATOM	2880	O	PHE	B	91	61.258	-10.892	7.578	1.00	25.55	8
	ATOM	2881	CB	PHE	B	91	58.346	-11.073	7.207	1.00	20.44	6
	ATOM	2882	CG	PHE	B	91	58.180	-10.275	5.969	1.00	22.85	6
30	ATOM	2883	CD1	PHE	B	91	58.030	-10.779	4.676	1.00	21.26	6
	ATOM	2884	CD2	PHE	B	91	58.164	-8.848	6.101	1.00	22.68	6
	ATOM	2885	CE1	PHE	B	91	57.900	-9.976	3.571	1.00	22.13	6
	ATOM	2886	CE2	PHE	B	91	58.006	-8.055	4.990	1.00	21.70	6
	ATOM	2887	CZ	PHE	B	91	57.852	-8.587	3.703	1.00	23.17	6
35	ATOM	2888	N	ALA	B	92	61.345	-12.164	5.695	1.00	24.62	7
	ATOM	2889	CA	ALA	B	92	62.738	-11.659	5.375	1.00	23.61	6
	ATOM	2890	C	ALA	B	92	62.815	-11.216	3.975	1.00	25.99	6
	ATOM	2891	O	ALA	B	92	63.216	-12.052	3.123	1.00	27.84	8
	ATOM	2892	CB	ALA	B	92	63.656	-12.811	5.743	1.00	25.77	6
40	ATOM	2893	N	PRO	B	93	62.300	-10.088	3.518	1.00	25.21	7
	ATOM	2894	CA	PRO	B	93	62.258	-9.655	2.170	1.00	26.28	6
	ATOM	2895	C	PRO	B	93	63.583	-9.189	1.617	1.00	25.56	6
	ATOM	2896	O	PRO	B	93	64.455	-8.761	2.381	1.00	27.95	8
	ATOM	2897	CB	PRO	B	93	61.283	-8.471	2.238	1.00	26.93	6
45	ATOM	2898	CG	PRO	B	93	61.547	-7.888	3.586	1.00	26.11	6
	ATOM	2899	CD	PRO	B	93	61.769	-9.060	4.516	1.00	24.38	6
	ATOM	2900	N	SER	B	94	63.668	-9.114	0.292	1.00	28.86	7
	ATOM	2901	CA	SER	B	94	64.891	-8.524	-0.309	1.00	30.21	6
	ATOM	2902	C	SER	B	94	64.735	-7.010	-0.305	1.00	31.63	6
50	ATOM	2903	O	SER	B	94	63.635	-6.521	-0.100	1.00	27.09	8
	ATOM	2904	CB	SER	B	94	65.138	-8.951	-1.719	1.00	28.52	6
	ATOM	2905	OG	SER	B	94	64.254	-8.353	-2.673	1.00	29.83	8
	ATOM	2906	N	VAL	B	95	65.802	-6.264	-0.628	1.00	32.49	7
	ATOM	2907	CA	VAL	B	95	65.724	-4.840	-0.723	1.00	31.55	6
55	ATOM	2908	C	VAL	B	95	64.919	-4.487	-1.938	1.00	31.75	6
	ATOM	2909	O	VAL	B	95	64.138	-3.540	-1.883	1.00	31.41	8
	ATOM	2910	CB	VAL	B	95	67.144	-4.172	-0.780	1.00	32.74	6
	ATOM	2911	CG1	VAL	B	95	67.050	-2.736	-1.221	1.00	34.17	6
	ATOM	2912	CG2	VAL	B	95	67.813	-4.258	0.570	1.00	33.43	6
60	ATOM	2913	N	LYS	B	96	65.004	-5.262	-3.023	1.00	31.26	7
	ATOM	2914	CA	LYS	B	96	64.226	-5.022	-4.212	1.00	31.62	6
	ATOM	2915	C	LYS	B	96	62.744	-5.267	-3.889	1.00	29.22	6
	ATOM	2916	O	LYS	B	96	61.905	-4.611	-4.487	1.00	32.48	8
	ATOM	2917	CB	LYS	B	96	64.685	-5.913	-5.380	1.00	32.35	6
65	ATOM	2918	N	GLU	B	97	62.464	-6.172	-2.988	1.00	30.27	7
	ATOM	2919	CA	GLU	B	97	61.056	-6.463	-2.667	1.00	31.03	6
	ATOM	2920	C	GLU	B	97	60.375	-5.301	-1.936	1.00	30.11	6
	ATOM	2921	O	GLU	B	97	59.235	-4.950	-2.211	1.00	31.04	8
	ATOM	2922	CB	GLU	B	97	61.000	-7.749	-1.850	1.00	32.49	6
70	ATOM	2923	CG	GLU	B	97	59.570	-8.220	-1.623	1.00	33.54	6
	ATOM	2924	CD	GLU	B	97	58.875	-8.792	-2.844	1.00	35.26	6
	ATOM	2925	OE1	GLU	B	97	59.540	-9.132	-3.867	1.00	34.07	8
	ATOM	2926	OE2	GLU	B	97	57.632	-8.980	-2.841	1.00	32.87	8
	ATOM	2927	N	ILE	B	98	61.084	-4.723	-0.999	1.00	28.92	7
	ATOM	2928	CA	ILE	B	98	60.582	-3.564	-0.235	1.00	28.98	6

-76-

	ATOM	2929	C	ILE	B	98	60.727	-2.241	-0.955	1.00	30.40	6
	ATOM	2930	O	ILE	B	98	59.849	-1.353	-0.964	1.00	25.83	8
	ATOM	2931	CB	ILE	B	98	61.320	-3.544	1.123	1.00	26.40	6
5	ATOM	2932	CG1	ILE	B	98	60.992	-4.753	1.985	1.00	30.78	6
	ATOM	2933	CG2	ILE	B	98	60.988	-2.241	1.865	1.00	26.02	6
	ATOM	2934	CD1	ILE	B	98	59.551	-5.137	2.182	1.00	30.67	6
	ATOM	2935	N	TYR	B	99	61.889	-2.036	-1.638	1.00	31.00	7
	ATOM	2936	CA	TYR	B	99	62.170	-0.808	-2.356	1.00	32.52	6
10	ATOM	2937	C	TYR	B	99	62.505	-1.034	-3.812	1.00	34.54	6
	ATOM	2938	O	TYR	B	99	63.655	-0.817	-4.255	1.00	35.45	8
	ATOM	2939	CB	TYR	B	99	63.366	-0.108	-1.661	1.00	31.16	6
	ATOM	2940	CG	TYR	B	99	63.179	0.250	-0.213	1.00	28.25	6
	ATOM	2941	CD1	TYR	B	99	63.952	-0.243	0.825	1.00	28.01	6
15	ATOM	2942	CD2	TYR	B	99	62.202	1.193	0.117	1.00	28.98	6
	ATOM	2943	CE1	TYR	B	99	63.754	0.159	2.135	1.00	27.92	6
	ATOM	2944	CE2	TYR	B	99	62.006	1.609	1.427	1.00	28.86	6
	ATOM	2945	CZ	TYR	B	99	62.774	1.073	2.446	1.00	27.90	6
	ATOM	2946	OH	TYR	B	99	62.576	1.499	3.756	1.00	27.84	8
20	ATOM	2947	N	PRO	B	100	61.555	-1.416	-4.630	1.00	35.55	7
	ATOM	2948	CA	PRO	B	100	61.774	-1.742	-6.033	1.00	37.21	6
	ATOM	2949	C	PRO	B	100	62.327	-0.598	-6.843	1.00	38.72	6
	ATOM	2950	O	PRO	B	100	63.107	-0.784	-7.787	1.00	39.39	8
	ATOM	2951	CB	PRO	B	100	60.417	-2.189	-6.566	1.00	37.99	6
25	ATOM	2952	CG	PRO	B	100	59.412	-1.828	-5.543	1.00	35.50	6
	ATOM	2953	CD	PRO	B	100	60.151	-1.710	-4.256	1.00	35.06	6
	ATOM	2954	N	ASN	B	101	61.921	0.620	-6.487	1.00	38.14	7
	ATOM	2955	CA	ASN	B	101	62.391	1.803	-7.192	1.00	38.05	6
	ATOM	2956	C	ASN	B	101	63.459	2.537	-6.385	1.00	36.99	6
30	ATOM	2957	O	ASN	B	101	63.676	3.726	-6.653	1.00	39.29	8
	ATOM	2958	CB	ASN	B	101	61.202	2.723	-7.451	1.00	39.89	6
	ATOM	2959	CG	ASN	B	101	60.007	1.987	-8.013	1.00	41.77	6
	ATOM	2960	OD1	ASN	B	101	58.930	1.884	-7.425	1.00	42.16	8
	ATOM	2961	ND2	ASN	B	101	60.229	1.436	-9.197	1.00	42.54	7
35	ATOM	2962	N	GLY	B	102	64.028	1.920	-5.376	1.00	34.24	7
	ATOM	2963	CA	GLY	B	102	64.956	2.603	-4.480	1.00	33.96	6
	ATOM	2964	C	GLY	B	102	64.329	3.353	-3.324	1.00	34.73	6
	ATOM	2965	O	GLY	B	102	63.091	3.507	-3.190	1.00	33.28	8
	ATOM	2966	N	THR	B	103	65.153	3.914	-2.430	1.00	32.52	7
40	ATOM	2967	CA	THR	B	103	64.591	4.613	-1.279	1.00	32.04	6
	ATOM	2968	C	THR	B	103	64.351	6.098	-1.472	1.00	33.64	6
	ATOM	2969	O	THR	B	103	63.426	6.615	-0.800	1.00	32.63	8
	ATOM	2970	CB	THR	B	103	65.544	4.405	-0.100	1.00	34.27	6
	ATOM	2971	OG1	THR	B	103	66.808	4.981	-0.489	1.00	34.81	8
45	ATOM	2972	CG2	THR	B	103	65.762	2.948	0.225	1.00	34.11	6
	ATOM	2973	N	GLU	B	104	65.063	6.775	-2.375	1.00	31.00	7
	ATOM	2974	CA	GLU	B	104	64.919	8.220	-2.452	1.00	34.38	6
	ATOM	2975	C	GLU	B	104	63.553	8.693	-2.915	1.00	35.05	6
	ATOM	2976	O	GLU	B	104	63.205	9.837	-2.567	1.00	36.53	8
50	ATOM	2977	CB	GLU	B	104	66.012	8.810	-3.394	1.00	37.66	6
	ATOM	2978	N	THR	B	105	62.883	7.955	-3.798	1.00	32.50	7
	ATOM	2979	CA	THR	B	105	61.572	8.395	-4.264	1.00	33.06	6
	ATOM	2980	C	THR	B	105	60.409	7.607	-3.633	1.00	30.67	6
	ATOM	2981	O	THR	B	105	59.255	7.825	-4.025	1.00	30.32	8
55	ATOM	2982	CB	THR	B	105	61.469	8.256	-5.780	1.00	34.96	6
	ATOM	2983	OG1	THR	B	105	61.702	6.883	-6.107	1.00	35.88	8
	ATOM	2984	CG2	THR	B	105	62.498	9.147	-6.493	1.00	37.41	6
	ATOM	2985	N	HIS	B	106	60.705	6.829	-2.610	1.00	28.38	7
	ATOM	2986	CA	HIS	B	106	59.686	6.055	-1.897	1.00	26.95	6
60	ATOM	2987	C	HIS	B	106	58.943	6.945	-0.916	1.00	27.21	6
	ATOM	2988	O	HIS	B	106	59.558	7.820	-0.286	1.00	25.40	8
	ATOM	2989	CB	HIS	B	106	60.299	4.906	-1.129	1.00	26.76	6
	ATOM	2990	CG	HIS	B	106	59.397	3.804	-0.619	1.00	26.50	6
	ATOM	2991	ND1	HIS	B	106	58.822	3.908	0.632	1.00	26.30	7
65	ATOM	2992	CD2	HIS	B	106	59.017	2.642	-1.214	1.00	26.99	6
	ATOM	2993	CE1	HIS	B	106	58.139	2.730	0.807	1.00	26.31	6
	ATOM	2994	NE2	HIS	B	106	58.209	1.992	-0.276	1.00	27.12	7
	ATOM	2995	N	THR	B	107	57.621	6.749	-0.815	1.00	24.60	7
	ATOM	2996	CA	THR	B	107	56.852	7.517	0.177	1.00	22.48	6
70	ATOM	2997	C	THR	B	107	57.510	7.428	1.528	1.00	23.26	6
	ATOM	2998	O	THR	B	107	58.100	6.378	1.812	1.00	24.71	8
	ATOM	2999	CB	THR	B	107	55.425	6.933	0.229	1.00	22.11	6
	ATOM	3000	OG1	THR	B	107	54.846	7.149	-1.052	1.00	21.94	8
	ATOM	3001	CG2	THR	B	107	54.603	7.713	1.242	1.00	24.08	6
	ATOM	3002	N	TYR	B	108	57.441	8.470	2.356	1.00	21.20	7

-77-

	ATOM	3003	CA	TYR	B	108	58.037	8.298	3.677	1.00	22.80	6
	ATOM	3004	C	TYR	B	108	57.170	8.870	4.799	1.00	23.19	6
	ATOM	3005	O	TYR	B	108	56.257	9.711	4.564	1.00	20.67	8
	ATOM	3006	CB	TYR	B	108	59.500	8.861	3.752	1.00	26.29	6
5	ATOM	3007	CG	TYR	B	108	59.581	10.367	3.586	1.00	27.43	6
	ATOM	3008	CD1	TYR	B	108	59.350	11.243	4.641	1.00	30.64	6
	ATOM	3009	CD2	TYR	B	108	59.795	10.914	2.331	1.00	31.95	6
	ATOM	3010	CE1	TYR	B	108	59.352	12.617	4.478	1.00	31.91	6
	ATOM	3011	CE2	TYR	B	108	59.821	12.272	2.159	1.00	34.14	6
10	ATOM	3012	CZ	TYR	B	108	59.609	13.130	3.235	1.00	34.42	6
	ATOM	3013	OH	TYR	B	108	59.634	14.497	3.014	1.00	36.77	8
	ATOM	3014	N	VAL	B	109	57.454	8.419	6.031	1.00	21.49	7
	ATOM	3015	CA	VAL	B	109	56.734	8.809	7.224	1.00	21.55	6
	ATOM	3016	C	VAL	B	109	57.707	9.552	8.149	1.00	23.45	6
15	ATOM	3017	O	VAL	B	109	58.712	8.918	8.447	1.00	22.21	8
	ATOM	3018	CB	VAL	B	109	56.125	7.624	8.009	1.00	20.74	6
	ATOM	3019	CG1	VAL	B	109	55.351	8.074	9.216	1.00	22.40	6
	ATOM	3020	CG2	VAL	B	109	55.248	6.829	7.006	1.00	21.59	6
	ATOM	3021	N	ASP	B	110	57.376	10.750	8.596	1.00	22.01	7
20	ATOM	3022	CA	ASP	B	110	58.343	11.465	9.478	1.00	24.43	6
	ATOM	3023	C	ASP	B	110	57.632	11.952	10.711	1.00	23.59	6
	ATOM	3024	O	ASP	B	110	56.504	12.458	10.672	1.00	21.44	8
	ATOM	3025	CB	ASP	B	110	58.991	12.648	8.759	1.00	27.76	6
	ATOM	3026	CG	ASP	B	110	60.461	12.751	9.239	1.00	36.19	6
25	ATOM	3027	OD1	ASP	B	110	61.056	12.013	10.077	1.00	37.59	8
	ATOM	3028	OD2	ASP	B	110	61.173	13.585	8.645	1.00	39.38	8
	ATOM	3029	N	VAL	B	111	58.257	11.795	11.892	1.00	23.56	7
	ATOM	3030	CA	VAL	B	111	57.669	12.175	13.148	1.00	22.23	6
	ATOM	3031	C	VAL	B	111	58.397	13.444	13.636	1.00	26.13	6
30	ATOM	3032	O	VAL	B	111	59.555	13.322	13.987	1.00	27.27	8
	ATOM	3033	CB	VAL	B	111	57.822	11.100	14.216	1.00	23.73	6
	ATOM	3034	CG1	VAL	B	111	57.213	11.440	15.574	1.00	23.64	6
	ATOM	3035	CG2	VAL	B	111	57.143	9.759	13.858	1.00	24.27	6
35	ATOM	3036	N	PRO	B	112	57.801	14.619	13.564	1.00	24.70	7
	ATOM	3037	CA	PRO	B	112	58.542	15.820	13.939	1.00	24.12	6
	ATOM	3038	C	PRO	B	112	59.048	15.823	15.355	1.00	25.44	6
	ATOM	3039	O	PRO	B	112	58.457	15.302	16.281	1.00	25.94	8
	ATOM	3040	CB	PRO	B	112	57.517	16.950	13.719	1.00	26.49	6
	ATOM	3041	CG	PRO	B	112	56.471	16.411	12.776	1.00	25.85	6
40	ATOM	3042	CD	PRO	B	112	56.449	14.912	13.005	1.00	25.31	6
	ATOM	3043	N	GLY	B	113	60.180	16.517	15.580	1.00	27.49	7
	ATOM	3044	CA	GLY	B	113	60.648	16.709	16.978	1.00	27.16	6
	ATOM	3045	C	GLY	B	113	61.466	15.490	17.404	1.00	29.14	6
	ATOM	3046	O	GLY	B	113	62.690	15.588	17.383	1.00	29.51	8
45	ATOM	3047	N	LEU	B	114	60.785	14.355	17.638	1.00	27.78	7
	ATOM	3048	CA	LEU	B	114	61.512	13.141	18.019	1.00	28.34	6
	ATOM	3049	C	LEU	B	114	62.545	12.685	17.019	1.00	29.38	6
	ATOM	3050	O	LEU	B	114	63.611	12.122	17.362	1.00	28.08	8
50	ATOM	3051	CB	LEU	B	114	60.493	12.006	18.279	1.00	26.74	6
	ATOM	3052	CG	LEU	B	114	59.539	12.250	19.424	1.00	28.28	6
	ATOM	3053	CD1	LEU	B	114	58.565	11.088	19.594	1.00	26.02	6
	ATOM	3054	CD2	LEU	B	114	60.295	12.476	20.742	1.00	28.90	6
	ATOM	3055	N	SER	B	115	62.355	12.921	15.738	1.00	28.55	7
	ATOM	3056	CA	SER	B	115	63.262	12.446	14.710	1.00	28.22	6
55	ATOM	3057	C	SER	B	115	64.540	13.284	14.611	1.00	30.73	6
	ATOM	3058	O	SER	B	115	65.515	12.778	14.048	1.00	29.82	8
	ATOM	3059	CB	SER	B	115	62.556	12.433	13.359	1.00	28.87	6
	ATOM	3060	OG	SER	B	115	62.188	13.728	12.878	1.00	31.15	8
60	ATOM	3061	N	THR	B	116	64.480	14.501	15.168	1.00	30.45	7
	ATOM	3062	CA	THR	B	116	65.625	15.383	14.934	1.00	32.38	6
	ATOM	3063	C	THR	B	116	66.349	15.755	16.226	1.00	34.29	6
	ATOM	3064	O	THR	B	116	67.346	16.447	16.085	1.00	38.91	8
	ATOM	3065	CB	THR	B	116	65.213	16.700	14.232	1.00	32.70	6
65	ATOM	3066	OG1	THR	B	116	64.062	17.200	14.921	1.00	32.18	8
	ATOM	3067	CG2	THR	B	116	64.868	16.509	12.776	1.00	33.85	6
	ATOM	3068	N	MET	B	117	65.882	15.315	17.364	1.00	34.18	7
	ATOM	3069	CA	MET	B	117	66.556	15.577	18.625	1.00	35.31	6
	ATOM	3070	C	MET	B	117	67.520	14.454	18.990	1.00	37.27	6
	ATOM	3071	O	MET	B	117	67.419	13.329	18.506	1.00	35.45	8
70	ATOM	3072	CB	MET	B	117	65.555	15.716	19.758	1.00	36.44	6
	ATOM	3073	CG	MET	B	117	64.825	14.432	20.149	1.00	34.64	6
	ATOM	3074	SD	MET	B	117	63.385	14.720	21.138	1.00	35.68	16
	ATOM	3075	CE	MET	B	117	64.113	15.441	22.628	1.00	35.24	6
	ATOM	3076	N	LEU	B	118	68.432	14.767	19.943	1.00	36.08	7

-78-

	ATOM	3077	CA	LEU	B	118	69.384	13.776	20.444	1.00	35.32	6
	ATOM	3078	C	LEU	B	118	70.141	13.060	19.370	1.00	36.49	6
	ATOM	3079	O	LEU	B	118	70.769	13.672	18.490	1.00	38.03	8
5	ATOM	3080	CB	LEU	B	118	68.602	12.780	21.326	1.00	34.52	6
	ATOM	3081	CG	LEU	B	118	67.955	13.401	22.550	1.00	34.53	6
	ATOM	3082	CD1	LEU	B	118	67.125	12.422	23.336	1.00	33.90	6
	ATOM	3083	CD2	LEU	B	118	69.054	13.987	23.492	1.00	36.09	6
	ATOM	3084	N	GLU	B	119	70.061	11.719	19.302	1.00	39.19	7
10	ATOM	3085	CA	GLU	B	119	70.748	10.969	18.252	1.00	39.90	6
	ATOM	3086	C	GLU	B	119	70.345	11.391	16.861	1.00	39.96	6
	ATOM	3087	O	GLU	B	119	71.144	11.319	15.930	1.00	39.74	8
	ATOM	3088	CB	GLU	B	119	70.439	9.477	18.447	1.00	42.37	6
	ATOM	3089	CG	GLU	B	119	71.094	8.560	17.433	1.00	46.28	6
15	ATOM	3090	CD	GLU	B	119	70.981	7.080	17.777	1.00	47.62	6
	ATOM	3091	OE1	GLU	B	119	70.337	6.733	18.805	1.00	48.65	8
	ATOM	3092	OE2	GLU	B	119	71.561	6.302	16.970	1.00	49.17	8
	ATOM	3093	N	GLY	B	120	69.102	11.892	16.668	1.00	38.75	7
	ATOM	3094	CA	GLY	B	120	68.668	12.258	15.318	1.00	39.65	6
20	ATOM	3095	C	GLY	B	120	69.318	13.524	14.807	1.00	41.25	6
	ATOM	3096	O	GLY	B	120	69.425	13.755	13.602	1.00	39.83	8
	ATOM	3097	N	ALA	B	121	69.785	14.354	15.771	1.00	42.58	7
	ATOM	3098	CA	ALA	B	121	70.410	15.623	15.404	1.00	44.15	6
	ATOM	3099	C	ALA	B	121	71.647	15.421	14.552	1.00	44.51	6
25	ATOM	3100	O	ALA	B	121	71.836	16.162	13.587	1.00	46.30	8
	ATOM	3101	CB	ALA	B	121	70.755	16.396	16.671	1.00	44.12	6
	ATOM	3102	N	SER	B	122	72.464	14.428	14.839	1.00	46.51	7
	ATOM	3103	CA	SER	B	122	73.663	14.179	14.040	1.00	48.95	6
	ATOM	3104	C	SER	B	122	73.442	13.166	12.932	1.00	49.98	6
30	ATOM	3105	O	SER	B	122	74.351	12.912	12.125	1.00	49.74	8
	ATOM	3106	CB	SER	B	122	74.790	13.675	14.943	1.00	49.52	6
	ATOM	3107	OG	SER	B	122	74.248	12.758	15.879	1.00	51.88	8
	ATOM	3108	N	ARG	B	123	72.222	12.591	12.854	1.00	48.32	7
	ATOM	3109	CA	ARG	B	123	71.947	11.586	11.826	1.00	46.67	6
35	ATOM	3110	C	ARG	B	123	70.694	11.919	11.018	1.00	46.85	6
	ATOM	3111	O	ARG	B	123	69.644	11.274	11.155	1.00	45.46	8
	ATOM	3112	CB	ARG	B	123	71.789	10.202	12.467	1.00	46.37	6
	ATOM	3113	CG	ARG	B	123	72.838	9.776	13.470	1.00	46.42	6
	ATOM	3114	CD	ARG	B	123	72.773	8.316	13.871	1.00	46.50	6
40	ATOM	3115	NE	ARG	B	123	72.926	7.465	12.686	1.00	47.12	7
	ATOM	3116	CZ	ARG	B	123	72.709	6.151	12.722	1.00	48.23	6
	ATOM	3117	NH1	ARG	B	123	72.343	5.594	13.870	1.00	48.08	7
	ATOM	3118	NH2	ARG	B	123	72.847	5.460	11.600	1.00	48.83	7
	ATOM	3119	N	PRO	B	124	70.814	12.888	10.125	1.00	46.75	7
45	ATOM	3120	CA	PRO	B	124	69.724	13.307	9.272	1.00	45.09	6
	ATOM	3121	C	PRO	B	124	69.159	12.130	8.501	1.00	43.72	6
	ATOM	3122	O	PRO	B	124	69.907	11.332	7.919	1.00	42.42	8
	ATOM	3123	CB	PRO	B	124	70.287	14.368	8.344	1.00	46.93	6
	ATOM	3124	CG	PRO	B	124	71.771	14.278	8.490	1.00	47.37	6
50	ATOM	3125	CD	PRO	B	124	72.023	13.715	9.861	1.00	46.92	6
	ATOM	3126	N	GLY	B	125	67.828	12.007	8.537	1.00	41.20	7
	ATOM	3127	CA	GLY	B	125	67.230	10.900	7.774	1.00	39.29	6
	ATOM	3128	C	GLY	B	125	67.135	9.577	8.510	1.00	37.20	6
	ATOM	3129	O	GLY	B	125	66.420	8.699	7.989	1.00	36.11	8
55	ATOM	3130	N	HIS	B	126	67.837	9.368	9.601	1.00	34.73	7
	ATOM	3131	CA	HIS	B	126	67.849	8.102	10.308	1.00	33.50	6
	ATOM	3132	C	HIS	B	126	66.493	7.708	10.877	1.00	32.20	6
	ATOM	3133	O	HIS	B	126	65.982	6.611	10.531	1.00	31.89	8
	ATOM	3134	CB	HIS	B	126	68.894	8.136	11.442	1.00	32.39	6
60	ATOM	3135	CG	HIS	B	126	68.767	6.907	12.285	1.00	30.02	6
	ATOM	3136	ND1	HIS	B	126	69.142	5.669	11.764	1.00	32.16	7
	ATOM	3137	CD2	HIS	B	126	68.315	6.679	13.524	1.00	28.99	6
	ATOM	3138	CE1	HIS	B	126	68.928	4.739	12.670	1.00	30.29	6
	ATOM	3139	NE2	HIS	B	126	68.411	5.323	13.726	1.00	31.28	7
65	ATOM	3140	N	PHE	B	127	65.874	8.567	11.680	1.00	28.23	7
	ATOM	3141	CA	PHE	B	127	64.599	8.199	12.287	1.00	27.72	6
	ATOM	3142	C	PHE	B	127	63.495	8.234	11.213	1.00	26.35	6
	ATOM	3143	O	PHE	B	127	62.599	7.393	11.386	1.00	26.75	8
	ATOM	3144	CB	PHE	B	127	64.268	9.034	13.528	1.00	27.25	6
70	ATOM	3145	CG	PHE	B	127	65.109	8.550	14.698	1.00	28.04	6
	ATOM	3146	CD1	PHE	B	127	66.034	9.472	15.239	1.00	27.72	6
	ATOM	3147	CD2	PHE	B	127	65.127	7.278	15.203	1.00	26.78	6
	ATOM	3148	CE1	PHE	B	127	66.838	9.035	16.291	1.00	26.75	6
	ATOM	3149	CE2	PHE	B	127	65.919	6.858	16.231	1.00	29.31	6
	ATOM	3150	CZ	PHE	B	127	66.844	7.755	16.771	1.00	26.94	6

-79-

	ATOM	3151	N	ARG	B	128	63.652	9.015	10.140	1.00	26.25	7
	ATOM	3152	CA	ARG	B	128	62.665	8.940	9.054	1.00	26.31	6
	ATOM	3153	C	ARG	B	128	62.641	7.529	8.474	1.00	27.01	6
5	ATOM	3154	O	ARG	B	128	61.607	6.896	8.176	1.00	27.70	8
	ATOM	3155	CB	ARG	B	128	62.995	9.950	7.986	1.00	29.81	6
	ATOM	3156	CG	ARG	B	128	62.174	9.865	6.694	1.00	28.97	6
	ATOM	3157	CD	ARG	B	128	62.614	10.959	5.713	1.00	31.50	6
	ATOM	3158	NE	ARG	B	128	62.199	12.249	6.307	1.00	36.12	7
10	ATOM	3159	CZ	ARG	B	128	62.359	13.422	5.685	1.00	36.94	6
	ATOM	3160	NH1	ARG	B	128	62.917	13.437	4.474	1.00	36.92	7
	ATOM	3161	NH2	ARG	B	128	61.956	14.553	6.237	1.00	36.80	7
	ATOM	3162	N	GLY	B	129	63.823	6.942	8.316	1.00	25.53	7
	ATOM	3163	CA	GLY	B	129	63.959	5.579	7.803	1.00	25.39	6
15	ATOM	3164	C	GLY	B	129	63.296	4.587	8.744	1.00	24.86	6
	ATOM	3165	O	GLY	B	129	62.618	3.654	8.238	1.00	24.05	8
	ATOM	3166	N	VAL	B	130	63.374	4.723	10.054	1.00	23.36	7
	ATOM	3167	CA	VAL	B	130	62.752	3.848	11.024	1.00	22.23	6
	ATOM	3168	C	VAL	B	130	61.208	3.977	10.944	1.00	23.73	6
20	ATOM	3169	O	VAL	B	130	60.528	2.931	10.910	1.00	21.98	8
	ATOM	3170	CB	VAL	B	130	63.156	4.153	12.443	1.00	24.21	6
	ATOM	3171	CG1	VAL	B	130	62.503	3.325	13.534	1.00	24.51	6
	ATOM	3172	CG2	VAL	B	130	64.713	3.953	12.537	1.00	24.12	6
	ATOM	3173	N	SER	B	131	60.667	5.199	11.057	1.00	21.64	7
25	ATOM	3174	CA	SER	B	131	59.218	5.336	11.014	1.00	21.18	6
	ATOM	3175	C	SER	B	131	58.706	4.864	9.647	1.00	21.42	6
	ATOM	3176	O	SER	B	131	57.608	4.304	9.684	1.00	22.71	8
	ATOM	3177	CB	SER	B	131	58.790	6.781	11.406	1.00	20.10	6
	ATOM	3178	OG	SER	B	131	59.534	7.744	10.678	1.00	22.33	8
30	ATOM	3179	N	THR	B	132	59.376	5.073	8.538	1.00	21.18	7
	ATOM	3180	CA	THR	B	132	58.883	4.600	7.250	1.00	22.97	6
	ATOM	3181	C	THR	B	132	58.795	3.079	7.224	1.00	25.11	6
	ATOM	3182	O	THR	B	132	57.728	2.514	6.885	1.00	19.95	8
	ATOM	3183	CB	THR	B	132	59.742	5.139	6.108	1.00	23.70	6
35	ATOM	3184	OG1	THR	B	132	59.721	6.590	6.182	1.00	21.14	8
	ATOM	3185	CG2	THR	B	132	59.214	4.628	4.749	1.00	21.10	6
	ATOM	3186	N	ILE	B	133	59.876	2.374	7.590	1.00	23.47	7
	ATOM	3187	CA	ILE	B	133	59.792	0.897	7.444	1.00	22.30	6
	ATOM	3188	C	ILE	B	133	58.868	0.339	8.499	1.00	20.08	6
40	ATOM	3189	O	ILE	B	133	58.186	-0.702	8.247	1.00	20.82	8
	ATOM	3190	CB	ILE	B	133	61.163	0.202	7.503	1.00	22.40	6
	ATOM	3191	CG1	ILE	B	133	61.076	-1.270	7.056	1.00	22.66	6
	ATOM	3192	CG2	ILE	B	133	61.699	0.252	8.924	1.00	22.72	6
	ATOM	3193	CD1	ILE	B	133	60.726	-1.465	5.594	1.00	24.76	6
45	ATOM	3194	N	VAL	B	134	58.775	0.887	9.716	1.00	19.44	7
	ATOM	3195	CA	VAL	B	134	57.874	0.272	10.678	1.00	19.92	6
	ATOM	3196	C	VAL	B	134	56.425	0.507	10.228	1.00	19.95	6
	ATOM	3197	O	VAL	B	134	55.596	-0.408	10.340	1.00	18.76	8
	ATOM	3198	CB	VAL	B	134	58.087	0.785	12.093	1.00	20.66	6
50	ATOM	3199	CG1	VAL	B	134	57.101	0.289	13.127	1.00	21.02	6
	ATOM	3200	CG2	VAL	B	134	59.472	0.315	12.628	1.00	23.22	6
	ATOM	3201	N	SER	B	135	56.098	1.693	9.701	1.00	21.84	7
	ATOM	3202	CA	SER	B	135	54.738	1.882	9.197	1.00	21.43	6
	ATOM	3203	C	SER	B	135	54.448	0.852	8.088	1.00	20.41	6
55	ATOM	3204	O	SER	B	135	53.335	0.320	8.054	1.00	19.83	8
	ATOM	3205	CB	SER	B	135	54.490	3.262	8.563	1.00	25.05	6
	ATOM	3206	OG	SER	B	135	54.496	4.192	9.637	1.00	30.48	8
	ATOM	3207	N	LYS	B	136	55.430	0.706	7.189	1.00	18.76	7
	ATOM	3208	CA	LYS	B	136	55.189	-0.267	6.067	1.00	20.34	6
60	ATOM	3209	C	LYS	B	136	54.944	-1.659	6.626	1.00	19.06	6
	ATOM	3210	O	LYS	B	136	54.010	-2.371	6.185	1.00	18.19	8
	ATOM	3211	CB	LYS	B	136	56.351	-0.243	5.052	1.00	20.12	6
	ATOM	3212	CG	LYS	B	136	56.143	-1.143	3.805	1.00	20.78	6
	ATOM	3213	CD	LYS	B	136	57.014	-0.638	2.664	1.00	22.99	6
65	ATOM	3214	CE	LYS	B	136	56.995	-1.594	1.478	1.00	25.34	6
	ATOM	3215	NZ	LYS	B	136	57.435	-0.897	0.229	1.00	25.62	7
	ATOM	3216	N	LEU	B	137	55.713	-2.120	7.604	1.00	17.80	7
	ATOM	3217	CA	LEU	B	137	55.582	-3.427	8.237	1.00	19.98	6
	ATOM	3218	C	LEU	B	137	54.275	-3.552	8.976	1.00	19.20	6
70	ATOM	3219	O	LEU	B	137	53.616	-4.573	8.857	1.00	18.56	8
	ATOM	3220	CB	LEU	B	137	56.745	-3.696	9.220	1.00	19.53	6
	ATOM	3221	CG	LEU	B	137	58.074	-4.009	8.556	1.00	22.60	6
	ATOM	3222	CD1	LEU	B	137	59.179	-3.990	9.627	1.00	18.94	6
	ATOM	3223	CD2	LEU	B	137	58.043	-5.360	7.886	1.00	20.42	6
	ATOM	3224	N	PHE	B	138	53.777	-2.469	9.583	1.00	16.81	7

-80-

	ATOM	3225	CA	PHE	B	138	52.487	-2.532	10.200	1.00	17.03	6
	ATOM	3226	C	PHE	B	138	51.342	-2.677	9.163	1.00	15.57	6
	ATOM	3227	O	PHE	B	138	50.365	-3.369	9.434	1.00	17.73	8
5	ATOM	3228	CB	PHE	B	138	52.183	-1.237	10.974	1.00	17.43	6
	ATOM	3229	CG	PHE	B	138	52.989	-1.110	12.277	1.00	18.89	6
	ATOM	3230	CD1	PHE	B	138	52.929	0.069	12.997	1.00	18.99	6
	ATOM	3231	CD2	PHE	B	138	53.729	-2.164	12.784	1.00	19.88	6
	ATOM	3232	CE1	PHE	B	138	53.604	0.229	14.200	1.00	18.80	6
10	ATOM	3233	CE2	PHE	B	138	54.411	-2.031	14.006	1.00	21.38	6
	ATOM	3234	CZ	PHE	B	138	54.324	-0.829	14.750	1.00	19.09	6
	ATOM	3235	N	ASN	B	139	51.457	-2.015	8.033	1.00	18.34	7
	ATOM	3236	CA	ASN	B	139	50.419	-2.157	7.032	1.00	17.77	6
	ATOM	3237	C	ASN	B	139	50.464	-3.511	6.357	1.00	18.27	6
15	ATOM	3238	O	ASN	B	139	49.403	-4.059	5.975	1.00	20.66	8
	ATOM	3239	CB	ASN	B	139	50.565	-1.044	5.974	1.00	19.21	6
	ATOM	3240	CG	ASN	B	139	50.220	0.335	6.571	1.00	23.72	6
	ATOM	3241	OD1	ASN	B	139	49.304	0.418	7.359	1.00	24.33	8
	ATOM	3242	ND2	ASN	B	139	50.901	1.344	6.090	1.00	25.57	7
20	ATOM	3243	N	LEU	B	140	51.670	-4.126	6.251	1.00	17.43	7
	ATOM	3244	CA	LEU	B	140	51.816	-5.435	5.643	1.00	19.77	6
	ATOM	3245	C	LEU	B	140	51.392	-6.531	6.585	1.00	21.88	6
	ATOM	3246	O	LEU	B	140	50.667	-7.465	6.154	1.00	22.03	8
	ATOM	3247	CB	LEU	B	140	53.291	-5.684	5.198	1.00	18.61	6
25	ATOM	3248	CG	LEU	B	140	53.850	-4.849	4.059	1.00	20.20	6
	ATOM	3249	CD1	LEU	B	140	55.377	-5.000	3.978	1.00	21.39	6
	ATOM	3250	CD2	LEU	B	140	53.219	-5.272	2.744	1.00	21.81	6
	ATOM	3251	N	VAL	B	141	51.714	-6.509	7.876	1.00	19.81	7
	ATOM	3252	CA	VAL	B	141	51.423	-7.589	8.813	1.00	19.15	6
30	ATOM	3253	C	VAL	B	141	50.129	-7.384	9.575	1.00	18.23	6
	ATOM	3254	O	VAL	B	141	49.508	-8.383	9.942	1.00	20.17	8
	ATOM	3255	CB	VAL	B	141	52.613	-7.729	9.811	1.00	18.50	6
	ATOM	3256	CG1	VAL	B	141	52.402	-8.790	10.886	1.00	19.99	6
	ATOM	3257	CG2	VAL	B	141	53.895	-8.020	9.003	1.00	21.20	6
35	ATOM	3258	N	GLN	B	142	49.697	-6.125	9.766	1.00	19.03	7
	ATOM	3259	CA	GLN	B	142	48.456	-5.803	10.496	1.00	18.67	6
	ATOM	3260	C	GLN	B	142	48.367	-6.472	11.813	1.00	18.44	6
	ATOM	3261	O	GLN	B	142	47.434	-7.193	12.153	1.00	18.66	8
40	ATOM	3262	CB	GLN	B	142	47.254	-6.242	9.585	1.00	23.65	6
	ATOM	3263	CG	GLN	B	142	47.341	-5.370	8.311	1.00	27.77	6
	ATOM	3264	CD	GLN	B	142	46.179	-5.714	7.395	1.00	31.08	6
	ATOM	3265	OE1	GLN	B	142	45.039	-5.391	7.745	1.00	34.74	8
	ATOM	3266	NE2	GLN	B	142	46.447	-6.335	6.281	1.00	33.99	7
	ATOM	3267	N	PRO	B	143	49.444	-6.363	12.645	1.00	19.66	7
45	ATOM	3268	CA	PRO	B	143	49.526	-7.003	13.913	1.00	21.32	6
	ATOM	3269	C	PRO	B	143	48.579	-6.373	14.939	1.00	20.88	6
	ATOM	3270	O	PRO	B	143	48.162	-5.222	14.777	1.00	23.53	8
	ATOM	3271	CB	PRO	B	143	50.974	-6.829	14.398	1.00	19.63	6
	ATOM	3272	CG	PRO	B	143	51.245	-5.445	13.833	1.00	20.10	6
50	ATOM	3273	CD	PRO	B	143	50.576	-5.419	12.433	1.00	20.21	6
	ATOM	3274	N	ASP	B	144	48.242	-7.127	15.964	1.00	19.65	7
	ATOM	3275	CA	ASP	B	144	47.481	-6.572	17.069	1.00	19.58	6
	ATOM	3276	C	ASP	B	144	48.443	-5.798	17.998	1.00	20.96	6
	ATOM	3277	O	ASP	B	144	48.078	-4.862	18.701	1.00	21.10	8
55	ATOM	3278	CB	ASP	B	144	46.769	-7.645	17.857	1.00	21.71	6
	ATOM	3279	CG	ASP	B	144	45.715	-8.336	16.977	1.00	29.09	6
	ATOM	3280	OD1	ASP	B	144	46.026	-9.413	16.419	1.00	28.54	8
	ATOM	3281	OD2	ASP	B	144	44.670	-7.652	16.763	1.00	29.74	8
	ATOM	3282	N	ILE	B	145	49.639	-6.395	18.133	1.00	19.56	7
60	ATOM	3283	CA	ILE	B	145	50.662	-5.948	19.117	1.00	20.94	6
	ATOM	3284	C	ILE	B	145	52.010	-5.887	18.446	1.00	19.85	6
	ATOM	3285	O	ILE	B	145	52.279	-6.676	17.481	1.00	19.52	8
	ATOM	3286	CB	ILE	B	145	50.680	-6.958	20.269	1.00	21.71	6
	ATOM	3287	CG1	ILE	B	145	49.386	-6.954	21.122	1.00	24.70	6
65	ATOM	3288	CG2	ILE	B	145	51.900	-6.729	21.173	1.00	26.93	6
	ATOM	3289	CD1	ILE	B	145	49.072	-8.328	21.695	1.00	28.80	6
	ATOM	3290	N	ALA	B	146	52.910	-4.978	18.807	1.00	20.13	7
	ATOM	3291	CA	ALA	B	146	54.247	-4.939	18.221	1.00	20.86	6
	ATOM	3292	C	ALA	B	146	55.243	-4.703	19.396	1.00	23.49	6
70	ATOM	3293	O	ALA	B	146	54.897	-3.879	20.234	1.00	21.46	8
	ATOM	3294	CB	ALA	B	146	54.442	-3.869	17.206	1.00	21.57	6
	ATOM	3295	N	CYS	B	147	56.282	-5.520	19.470	1.00	21.24	7
	ATOM	3296	CA	CYS	B	147	57.227	-5.418	20.634	1.00	21.57	6
	ATOM	3297	C	CYS	B	147	58.514	-4.835	20.232	1.00	19.68	6
	ATOM	3298	O	CYS	B	147	59.148	-5.086	19.189	1.00	23.55	8

-81-

	ATOM	3299	CB	CYS	B	147	57.487	-6.803	21.192	1.00	25.97	6
	ATOM	3300	SG	CYS	B	147	56.049	-7.649	21.811	1.00	30.41	16
	ATOM	3301	N	PHE	B	148	59.070	-3.904	21.116	1.00	21.36	7
	ATOM	3302	CA	PHE	B	148	60.268	-3.195	20.823	1.00	19.98	6
5	ATOM	3303	C	PHE	B	148	61.134	-3.123	22.146	1.00	19.23	6
	ATOM	3304	O	PHE	B	148	60.479	-3.140	23.148	1.00	23.93	8
	ATOM	3305	CB	PHE	B	148	60.072	-1.760	20.374	1.00	22.31	6
	ATOM	3306	CG	PHE	B	148	59.349	-1.636	19.056	1.00	21.62	6
10	ATOM	3307	CD1	PHE	B	148	57.968	-1.677	19.110	1.00	22.35	6
	ATOM	3308	CD2	PHE	B	148	60.045	-1.548	17.891	1.00	24.41	6
	ATOM	3309	CE1	PHE	B	148	57.226	-1.664	17.918	1.00	21.17	6
	ATOM	3310	CE2	PHE	B	148	59.307	-1.425	16.674	1.00	23.20	6
	ATOM	3311	CZ	PHE	B	148	57.930	-1.509	16.754	1.00	19.10	6
15	ATOM	3312	N	GLY	B	149	62.415	-3.168	22.002	1.00	22.90	7
	ATOM	3313	CA	GLY	B	149	63.243	-3.177	23.235	1.00	24.26	6
	ATOM	3314	C	GLY	B	149	63.315	-1.783	23.884	1.00	26.58	6
	ATOM	3315	O	GLY	B	149	63.397	-0.779	23.199	1.00	27.16	8
	ATOM	3316	N	GLU	B	150	63.380	-1.759	25.212	1.00	27.01	7
20	ATOM	3317	CA	GLU	B	150	63.530	-0.425	25.870	1.00	29.68	6
	ATOM	3318	C	GLU	B	150	64.894	0.200	25.737	1.00	31.07	6
	ATOM	3319	O	GLU	B	150	65.020	1.425	25.978	1.00	30.50	8
	ATOM	3320	CB	GLU	B	150	63.214	-0.532	27.368	1.00	31.68	6
	ATOM	3321	CG	GLU	B	150	61.747	-0.632	27.660	1.00	34.09	6
25	ATOM	3322	CD	GLU	B	150	61.359	-0.743	29.111	1.00	37.99	6
	ATOM	3323	OE1	GLU	B	150	62.205	-0.936	30.001	1.00	38.43	8
	ATOM	3324	OE2	GLU	B	150	60.143	-0.643	29.350	1.00	40.17	8
	ATOM	3325	N	LYS	B	151	65.951	-0.544	25.401	1.00	29.23	7
	ATOM	3326	CA	LYS	B	151	67.258	0.093	25.292	1.00	31.41	6
30	ATOM	3327	C	LYS	B	151	67.273	1.220	24.300	1.00	31.27	6
	ATOM	3328	O	LYS	B	151	67.936	2.260	24.433	1.00	27.21	8
	ATOM	3329	CB	LYS	B	151	68.320	-0.926	24.878	1.00	34.10	6
	ATOM	3330	CG	LYS	B	151	69.755	-0.397	24.923	1.00	37.66	6
	ATOM	3331	CD	LYS	B	151	70.640	-1.476	24.317	1.00	41.05	6
35	ATOM	3332	CE	LYS	B	151	72.080	-1.431	24.765	1.00	43.98	6
	ATOM	3333	NZ	LYS	B	151	72.893	-0.452	23.975	1.00	44.59	7
	ATOM	3334	N	ASP	B	152	66.506	1.027	23.164	1.00	28.39	7
	ATOM	3335	CA	ASP	B	152	66.518	2.032	22.110	1.00	28.38	6
	ATOM	3336	C	ASP	B	152	65.332	2.937	22.374	1.00	28.23	6
40	ATOM	3337	O	ASP	B	152	64.210	2.803	21.783	1.00	26.26	8
	ATOM	3338	CB	ASP	B	152	66.440	1.375	20.725	1.00	28.61	6
	ATOM	3339	N	PHE	B	153	65.516	3.702	23.467	1.00	25.07	7
	ATOM	3340	CA	PHE	B	153	64.373	4.471	23.974	1.00	26.53	6
	ATOM	3341	C	PHE	B	153	63.892	5.520	22.974	1.00	21.61	6
45	ATOM	3342	O	PHE	B	153	62.708	5.839	23.024	1.00	24.77	8
	ATOM	3343	CB	PHE	B	153	64.730	5.118	25.330	1.00	26.51	6
	ATOM	3344	CG	PHE	B	153	65.779	6.167	25.190	1.00	29.71	6
	ATOM	3345	CD1	PHE	B	153	65.443	7.493	24.943	1.00	29.96	6
	ATOM	3346	CD2	PHE	B	153	67.132	5.855	25.398	1.00	29.77	6
50	ATOM	3347	CE1	PHE	B	153	66.423	8.454	24.846	1.00	31.18	6
	ATOM	3348	CE2	PHE	B	153	68.099	6.820	25.256	1.00	28.84	6
	ATOM	3349	CZ	PHE	B	153	67.763	8.135	24.997	1.00	31.32	6
	ATOM	3350	N	GLN	B	154	64.740	6.002	22.113	1.00	23.01	7
	ATOM	3351	CA	GLN	B	154	64.352	7.012	21.149	1.00	24.58	6
55	ATOM	3352	C	GLN	B	154	63.443	6.353	20.075	1.00	24.87	6
	ATOM	3353	O	GLN	B	154	62.466	6.997	19.707	1.00	23.87	8
	ATOM	3354	CB	GLN	B	154	65.558	7.664	20.502	1.00	26.01	6
	ATOM	3355	CG	GLN	B	154	65.117	8.877	19.710	1.00	28.34	6
	ATOM	3356	CD	GLN	B	154	66.171	9.934	19.456	1.00	30.51	6
60	ATOM	3357	OE1	GLN	B	154	67.342	9.742	19.766	1.00	32.27	8
	ATOM	3358	NE2	GLN	B	154	65.742	11.030	18.839	1.00	28.70	7
	ATOM	3359	N	GLN	B	155	63.841	5.183	19.619	1.00	24.42	7
	ATOM	3360	CA	GLN	B	155	62.944	4.439	18.714	1.00	24.63	6
	ATOM	3361	C	GLN	B	155	61.612	4.204	19.382	1.00	22.70	6
65	ATOM	3362	O	GLN	B	155	60.577	4.285	18.652	1.00	24.30	8
	ATOM	3363	CB	GLN	B	155	63.549	3.094	18.268	1.00	25.06	6
	ATOM	3364	CG	GLN	B	155	64.450	3.209	17.029	1.00	29.61	6
	ATOM	3365	CD	GLN	B	155	64.506	1.856	16.285	1.00	32.67	6
	ATOM	3366	OE1	GLN	B	155	65.360	1.610	15.440	1.00	37.92	8
70	ATOM	3367	NE2	GLN	B	155	63.610	0.953	16.599	1.00	28.61	7
	ATOM	3368	N	LEU	B	156	61.522	3.748	20.602	1.00	20.20	7
	ATOM	3369	CA	LEU	B	156	60.288	3.409	21.273	1.00	22.81	6
	ATOM	3370	C	LEU	B	156	59.381	4.671	21.280	1.00	25.01	6
	ATOM	3371	O	LEU	B	156	58.192	4.596	20.961	1.00	22.03	8
	ATOM	3372	CB	LEU	B	156	60.549	2.887	22.651	1.00	23.28	6

-82-

	ATOM	3373	CG	LEU	B	156	59.393	2.429	23.497	1.00	22.55	6
	ATOM	3374	CD1	LEU	B	156	58.484	1.403	22.784	1.00	24.60	6
	ATOM	3375	CD2	LEU	B	156	59.895	1.814	24.812	1.00	24.72	6
5	ATOM	3376	N	ALA	B	157	59.971	5.799	21.745	1.00	21.98	7
	ATOM	3377	CA	ALA	B	157	59.149	7.006	21.699	1.00	23.16	6
	ATOM	3378	C	ALA	B	157	58.684	7.366	20.300	1.00	21.84	6
	ATOM	3379	O	ALA	B	157	57.504	7.836	20.225	1.00	22.95	8
	ATOM	3380	CB	ALA	B	157	59.953	8.235	22.216	1.00	21.48	6
10	ATOM	3381	N	LEU	B	158	59.510	7.286	19.278	1.00	20.55	7
	ATOM	3382	CA	LEU	B	158	59.209	7.601	17.902	1.00	24.17	6
	ATOM	3383	C	LEU	B	158	58.018	6.737	17.408	1.00	24.35	6
	ATOM	3384	O	LEU	B	158	57.063	7.345	16.896	1.00	21.76	8
	ATOM	3385	CB	LEU	B	158	60.387	7.347	16.959	1.00	23.67	6
15	ATOM	3386	CG	LEU	B	158	60.332	7.840	15.511	1.00	25.33	6
	ATOM	3387	CD1	LEU	B	158	60.910	9.254	15.385	1.00	25.04	6
	ATOM	3388	CD2	LEU	B	158	61.078	6.855	14.633	1.00	24.59	6
	ATOM	3389	N	ILE	B	159	58.085	5.451	17.683	1.00	21.94	7
	ATOM	3390	CA	ILE	B	159	56.938	4.578	17.235	1.00	22.18	6
20	ATOM	3391	C	ILE	B	159	55.685	4.727	18.032	1.00	24.01	6
	ATOM	3392	O	ILE	B	159	54.587	4.804	17.414	1.00	21.79	8
	ATOM	3393	CB	ILE	B	159	57.436	3.108	17.263	1.00	21.63	6
	ATOM	3394	CG1	ILE	B	159	58.615	3.036	16.314	1.00	21.10	6
	ATOM	3395	CG2	ILE	B	159	56.305	2.118	16.906	1.00	21.29	6
25	ATOM	3396	CD1	ILE	B	159	58.290	3.361	14.848	1.00	27.17	6
	ATOM	3397	N	ARG	B	160	55.764	5.016	19.357	1.00	21.20	7
	ATOM	3398	CA	ARG	B	160	54.563	5.304	20.113	1.00	23.22	6
	ATOM	3399	C	ARG	B	160	53.911	6.620	19.579	1.00	20.84	6
	ATOM	3400	O	ARG	B	160	52.688	6.604	19.482	1.00	22.99	8
30	ATOM	3401	CB	ARG	B	160	54.786	5.438	21.627	1.00	22.64	6
	ATOM	3402	CG	ARG	B	160	54.975	4.035	22.266	1.00	25.40	6
	ATOM	3403	CD	ARG	B	160	55.364	4.303	23.720	0.50	28.99	6
	ATOM	3404	NE	ARG	B	160	55.627	3.143	24.540	0.50	32.14	7
	ATOM	3405	CZ	ARG	B	160	54.843	2.116	24.819	0.50	32.06	6
35	ATOM	3406	NH1	ARG	B	160	53.609	1.993	24.361	0.50	31.32	7
	ATOM	3407	NH2	ARG	B	160	55.288	1.143	25.624	0.50	32.40	7
	ATOM	3408	N	LYS	B	161	54.699	7.617	19.257	1.00	20.06	7
	ATOM	3409	CA	LYS	B	161	54.121	8.866	18.707	1.00	19.89	6
	ATOM	3410	C	LYS	B	161	53.502	8.570	17.331	1.00	20.88	6
40	ATOM	3411	O	LYS	B	161	52.418	9.085	17.017	1.00	20.38	8
	ATOM	3412	CB	LYS	B	161	55.172	9.998	18.633	1.00	21.42	6
	ATOM	3413	CG	LYS	B	161	54.474	11.290	18.133	1.00	23.56	6
	ATOM	3414	CD	LYS	B	161	55.345	12.508	18.131	1.00	27.88	6
	ATOM	3415	CE	LYS	B	161	54.736	13.692	17.336	1.00	31.75	6
45	ATOM	3416	NZ	LYS	B	161	53.349	13.890	17.879	1.00	29.32	7
	ATOM	3417	N	MET	B	162	54.244	7.875	16.465	1.00	19.25	7
	ATOM	3418	CA	MET	B	162	53.744	7.586	15.106	1.00	20.25	6
	ATOM	3419	C	MET	B	162	52.443	6.849	15.190	1.00	20.77	6
	ATOM	3420	O	MET	B	162	51.432	7.100	14.451	1.00	20.50	8
50	ATOM	3421	CB	MET	B	162	54.864	6.798	14.378	1.00	20.27	6
	ATOM	3422	CG	MET	B	162	54.438	6.504	12.918	1.00	20.30	6
	ATOM	3423	SD	MET	B	162	55.575	5.209	12.231	1.00	23.99	16
	ATOM	3424	CE	MET	B	162	54.976	3.754	13.066	1.00	22.75	6
	ATOM	3425	N	VAL	B	163	52.331	5.858	16.110	1.00	19.38	7
55	ATOM	3426	CA	VAL	B	163	51.106	5.095	16.243	1.00	20.12	6
	ATOM	3427	C	VAL	B	163	49.926	5.955	16.693	1.00	22.03	6
	ATOM	3428	O	VAL	B	163	48.820	5.841	16.163	1.00	19.78	8
	ATOM	3429	CB	VAL	B	163	51.310	3.926	17.212	1.00	19.66	6
	ATOM	3430	CG1	VAL	B	163	50.044	3.269	17.672	1.00	20.89	6
60	ATOM	3431	CG2	VAL	B	163	52.253	2.958	16.455	1.00	20.73	6
	ATOM	3432	N	ALA	B	164	50.127	6.771	17.688	1.00	20.47	7
	ATOM	3433	CA	ALA	B	164	49.065	7.634	18.189	1.00	21.69	6
	ATOM	3434	C	ALA	B	164	48.642	8.624	17.101	1.00	20.50	6
	ATOM	3435	O	ALA	B	164	47.419	8.750	16.892	1.00	23.25	8
65	ATOM	3436	CB	ALA	B	164	49.604	8.359	19.418	1.00	20.80	6
	ATOM	3437	N	ASP	B	165	49.612	9.237	16.440	1.00	19.12	7
	ATOM	3438	CA	ASP	B	165	49.190	10.233	15.409	1.00	18.46	6
	ATOM	3439	C	ASP	B	165	48.550	9.577	14.207	1.00	22.82	6
	ATOM	3440	O	ASP	B	165	47.594	10.145	13.660	1.00	22.60	8
70	ATOM	3441	CB	ASP	B	165	50.392	10.996	14.943	1.00	18.70	6
	ATOM	3442	CG	ASP	B	165	51.018	12.009	15.941	1.00	18.80	6
	ATOM	3443	OD1	ASP	B	165	50.354	12.300	16.916	1.00	21.84	8
	ATOM	3444	OD2	ASP	B	165	52.112	12.486	15.692	1.00	21.56	8
	ATOM	3445	N	MET	B	166	49.185	8.526	13.694	1.00	19.28	7
	ATOM	3446	CA	MET	B	166	48.660	7.953	12.411	1.00	20.68	6

-83-

	ATOM	3447	C	MET	B	166	47.436	7.082	12.604	1.00	21.52	6
	ATOM	3448	O	MET	B	166	46.935	6.605	11.577	1.00	22.25	8
	ATOM	3449	CB	MET	B	166	49.878	7.292	11.723	1.00	17.15	6
	ATOM	3450	CG	MET	B	166	50.905	8.348	11.281	1.00	21.78	6
5	ATOM	3451	SD	MET	B	166	50.266	9.743	10.357	1.00	21.48	16
	ATOM	3452	CE	MET	B	166	49.315	9.048	8.969	1.00	22.58	6
	ATOM	3453	N	GLY	B	167	46.947	6.745	13.792	1.00	22.34	7
	ATOM	3454	CA	GLY	B	167	45.725	5.983	14.001	1.00	21.60	6
	ATOM	3455	C	GLY	B	167	45.804	4.480	13.881	1.00	21.23	6
10	ATOM	3456	O	GLY	B	167	44.803	3.783	13.677	1.00	19.88	8
	ATOM	3457	N	PHE	B	168	47.043	3.939	13.961	1.00	21.11	7
	ATOM	3458	CA	PHE	B	168	47.170	2.494	13.958	1.00	20.42	6
	ATOM	3459	C	PHE	B	168	46.553	1.828	15.193	1.00	20.83	6
	ATOM	3460	O	PHE	B	168	46.842	2.233	16.321	1.00	22.53	8
15	ATOM	3461	CB	PHE	B	168	48.653	2.079	13.921	1.00	21.51	6
	ATOM	3462	CG	PHE	B	168	49.420	2.244	12.648	1.00	21.26	6
	ATOM	3463	CD1	PHE	B	168	50.305	3.310	12.535	1.00	21.28	6
	ATOM	3464	CD2	PHE	B	168	49.352	1.351	11.604	1.00	21.16	6
	ATOM	3465	CE1	PHE	B	168	51.095	3.489	11.409	1.00	22.13	6
20	ATOM	3466	CE2	PHE	B	168	50.080	1.550	10.442	1.00	24.10	6
	ATOM	3467	CZ	PHE	B	168	50.978	2.592	10.348	1.00	20.59	6
	ATOM	3468	N	ASP	B	169	45.751	0.812	14.997	1.00	22.55	7
	ATOM	3469	CA	ASP	B	169	45.089	0.089	16.054	1.00	23.63	6
	ATOM	3470	C	ASP	B	169	46.010	-1.072	16.556	1.00	23.14	6
25	ATOM	3471	O	ASP	B	169	45.637	-2.215	16.493	1.00	23.77	8
	ATOM	3472	CB	ASP	B	169	43.773	-0.497	15.594	1.00	27.60	6
	ATOM	3473	CG	ASP	B	169	42.879	-1.031	16.711	1.00	30.74	6
	ATOM	3474	OD1	ASP	B	169	43.197	-0.784	17.892	1.00	34.41	8
	ATOM	3475	OD2	ASP	B	169	41.884	-1.685	16.342	1.00	34.81	8
30	ATOM	3476	N	ILE	B	170	47.137	-0.643	17.058	1.00	20.48	7
	ATOM	3477	CA	ILE	B	170	48.196	-1.584	17.457	1.00	19.43	6
	ATOM	3478	C	ILE	B	170	48.725	-1.236	18.834	1.00	21.42	6
	ATOM	3479	O	ILE	B	170	49.048	-0.083	19.071	1.00	22.91	8
	ATOM	3480	CB	ILE	B	170	49.351	-1.526	16.434	1.00	19.13	6
35	ATOM	3481	CG1	ILE	B	170	48.940	-1.849	14.994	1.00	21.06	6
	ATOM	3482	CG2	ILE	B	170	50.464	-2.519	16.854	1.00	20.00	6
	ATOM	3483	CD1	ILE	B	170	50.054	-1.568	13.974	1.00	23.10	6
	ATOM	3484	N	GLU	B	171	48.847	-2.233	19.720	1.00	20.51	7
	ATOM	3485	CA	GLU	B	171	49.415	-1.968	21.050	1.00	22.48	6
40	ATOM	3486	C	GLU	B	171	50.925	-1.992	20.961	1.00	23.14	6
	ATOM	3487	O	GLU	B	171	51.470	-3.024	20.518	1.00	23.79	8
	ATOM	3488	CB	GLU	B	171	48.824	-2.974	22.034	1.00	24.29	6
	ATOM	3489	CG	GLU	B	171	49.506	-2.861	23.391	1.00	28.59	6
	ATOM	3490	CD	GLU	B	171	49.089	-3.843	24.453	1.00	33.66	6
45	ATOM	3491	OE1	GLU	B	171	48.310	-4.782	24.246	1.00	34.21	8
	ATOM	3492	OE2	GLU	B	171	49.580	-3.608	25.609	1.00	37.13	8
	ATOM	3493	N	ILE	B	172	51.637	-0.956	21.410	1.00	21.22	7
	ATOM	3494	CA	ILE	B	172	53.093	-0.965	21.349	1.00	19.30	6
	ATOM	3495	C	ILE	B	172	53.656	-1.362	22.720	1.00	24.29	6
50	ATOM	3496	O	ILE	B	172	53.145	-0.847	23.730	1.00	25.41	8
	ATOM	3497	CB	ILE	B	172	53.631	0.401	20.893	1.00	20.79	6
	ATOM	3498	CG1	ILE	B	172	53.086	0.809	19.509	1.00	22.57	6
	ATOM	3499	CG2	ILE	B	172	55.162	0.435	20.888	1.00	22.05	6
	ATOM	3500	CD1	ILE	B	172	53.459	-0.175	18.386	1.00	21.95	6
55	ATOM	3501	N	VAL	B	173	54.392	-2.471	22.752	1.00	21.27	7
	ATOM	3502	CA	VAL	B	173	54.895	-3.034	24.024	1.00	25.99	6
	ATOM	3503	C	VAL	B	173	56.363	-2.785	24.113	1.00	25.58	6
	ATOM	3504	O	VAL	B	173	57.087	-3.255	23.240	1.00	22.50	8
	ATOM	3505	CB	VAL	B	173	54.583	-4.552	24.123	1.00	25.82	6
60	ATOM	3506	CG1	VAL	B	173	55.242	-5.122	25.406	1.00	26.85	6
	ATOM	3507	CG2	VAL	B	173	53.094	-4.779	24.096	1.00	27.94	6
	ATOM	3508	N	GLY	B	174	56.820	-2.085	25.189	1.00	24.62	7
	ATOM	3509	CA	GLY	B	174	58.270	-1.862	25.313	1.00	23.53	6
	ATOM	3510	C	GLY	B	174	58.740	-3.002	26.282	1.00	23.91	6
65	ATOM	3511	O	GLY	B	174	57.998	-3.288	27.218	1.00	26.78	8
	ATOM	3512	N	VAL	B	175	59.801	-3.641	25.849	1.00	22.58	7
	ATOM	3513	CA	VAL	B	175	60.234	-4.783	26.676	1.00	24.09	6
	ATOM	3514	C	VAL	B	175	61.523	-4.341	27.430	1.00	23.90	6
	ATOM	3515	O	VAL	B	175	62.502	-4.011	26.762	1.00	24.10	8
70	ATOM	3516	CB	VAL	B	175	60.476	-6.015	25.853	1.00	24.37	6
	ATOM	3517	CG1	VAL	B	175	60.852	-7.180	26.767	1.00	28.33	6
	ATOM	3518	CG2	VAL	B	175	59.219	-6.353	24.984	1.00	24.52	6
	ATOM	3519	N	PRO	B	176	61.469	-4.464	28.728	1.00	28.58	7
	ATOM	3520	CA	PRO	B	176	62.648	-4.211	29.574	1.00	32.47	6

-84-

	ATOM	3521	C	PRO	B	176	63.888	-4.974	29.180	1.00	32.41	6
	ATOM	3522	O	PRO	B	176	63.831	-6.135	28.746	1.00	28.92	8
	ATOM	3523	CB	PRO	B	176	62.159	-4.588	30.980	1.00	33.03	6
5	ATOM	3524	CG	PRO	B	176	60.685	-4.380	30.922	1.00	34.15	6
	ATOM	3525	CD	PRO	B	176	60.320	-4.916	29.543	1.00	28.09	6
	ATOM	3526	N	ILE	B	177	65.121	-4.418	29.353	1.00	31.48	7
	ATOM	3527	CA	ILE	B	177	66.307	-5.079	28.865	1.00	32.30	6
	ATOM	3528	C	ILE	B	177	66.572	-6.407	29.607	1.00	30.07	6
10	ATOM	3529	O	ILE	B	177	66.054	-6.698	30.686	1.00	32.04	8
	ATOM	3530	CB	ILE	B	177	67.641	-4.292	28.903	1.00	33.70	6
	ATOM	3531	CG1	ILE	B	177	68.066	-3.943	30.331	1.00	33.12	6
	ATOM	3532	CG2	ILE	B	177	67.518	-3.039	28.030	1.00	34.28	6
	ATOM	3533	CD1	ILE	B	177	69.430	-3.243	30.349	1.00	34.81	6
15	ATOM	3534	N	MET	B	178	67.408	-7.204	28.952	1.00	32.08	7
	ATOM	3535	CA	MET	B	178	67.674	-8.503	29.572	1.00	35.37	6
	ATOM	3536	C	MET	B	178	68.620	-8.292	30.772	1.00	34.12	6
	ATOM	3537	O	MET	B	178	69.597	-7.573	30.642	1.00	31.98	8
	ATOM	3538	CB	MET	B	178	68.295	-9.532	28.641	1.00	40.27	6
20	ATOM	3539	CG	MET	B	178	67.437	-10.819	28.679	1.00	44.21	6
	ATOM	3540	SD	MET	B	178	68.203	-12.124	27.749	1.00	51.85	16
	ATOM	3541	CE	MET	B	178	69.561	-11.316	26.916	1.00	48.86	6
	ATOM	3542	N	ARG	B	179	68.313	-8.994	31.814	1.00	35.69	7
	ATOM	3543	CA	ARG	B	179	69.085	-8.847	33.060	1.00	36.43	6
25	ATOM	3544	C	ARG	B	179	69.292	-10.188	33.715	1.00	37.86	6
	ATOM	3545	O	ARG	B	179	68.430	-11.054	33.618	1.00	38.23	8
	ATOM	3546	CB	ARG	B	179	68.260	-7.887	33.870	1.00	36.62	6
	ATOM	3547	CG	ARG	B	179	68.473	-7.248	35.163	1.00	38.40	6
	ATOM	3548	CD	ARG	B	179	67.373	-6.311	35.598	1.00	34.70	6
30	ATOM	3549	NE	ARG	B	179	67.202	-5.122	34.808	1.00	31.82	7
	ATOM	3550	CZ	ARG	B	179	68.057	-4.149	34.534	1.00	32.71	6
	ATOM	3551	NH1	ARG	B	179	69.308	-4.167	34.984	1.00	30.99	7
	ATOM	3552	NH2	ARG	B	179	67.715	-3.067	33.831	1.00	33.25	7
	ATOM	3553	N	ALA	B	180	70.363	-10.335	34.477	1.00	36.11	7
35	ATOM	3554	CA	ALA	B	180	70.602	-11.562	35.235	1.00	36.60	6
	ATOM	3555	C	ALA	B	180	69.640	-11.614	36.404	1.00	36.37	6
	ATOM	3556	O	ALA	B	180	68.929	-10.685	36.743	1.00	36.44	8
	ATOM	3557	CB	ALA	B	180	72.048	-11.541	35.689	1.00	36.08	6
	ATOM	3558	N	LYS	B	181	69.621	-12.775	37.102	1.00	37.25	7
40	ATOM	3559	CA	LYS	B	181	68.797	-12.903	38.292	1.00	38.41	6
	ATOM	3560	C	LYS	B	181	69.223	-11.942	39.395	1.00	37.82	6
	ATOM	3561	O	LYS	B	181	68.366	-11.482	40.158	1.00	40.11	8
	ATOM	3562	CB	LYS	B	181	68.862	-14.317	38.895	1.00	39.54	6
	ATOM	3563	N	ASP	B	182	70.495	-11.584	39.503	1.00	36.65	7
45	ATOM	3564	CA	ASP	B	182	70.935	-10.663	40.548	1.00	35.51	6
	ATOM	3565	C	ASP	B	182	70.714	-9.206	40.091	1.00	35.06	6
	ATOM	3566	O	ASP	B	182	71.004	-8.303	40.868	1.00	33.11	8
	ATOM	3567	CB	ASP	B	182	72.392	-10.861	40.981	1.00	37.04	6
	ATOM	3568	CG	ASP	B	182	73.414	-10.661	39.890	1.00	38.43	6
50	ATOM	3569	OD1	ASP	B	182	73.047	-10.265	38.753	1.00	38.66	8
	ATOM	3570	OD2	ASP	B	182	74.624	-10.938	40.116	1.00	38.45	8
	ATOM	3571	N	GLY	B	183	70.283	-8.992	38.840	1.00	35.23	7
	ATOM	3572	CA	GLY	B	183	69.907	-7.618	38.467	1.00	32.81	6
	ATOM	3573	C	GLY	B	183	70.883	-7.003	37.494	1.00	33.61	6
55	ATOM	3574	O	GLY	B	183	70.523	-5.956	36.928	1.00	33.06	8
	ATOM	3575	N	LEU	B	184	72.029	-7.592	37.220	1.00	31.99	7
	ATOM	3576	CA	LEU	B	184	72.977	-7.004	36.286	1.00	32.29	6
	ATOM	3577	C	LEU	B	184	72.517	-7.011	34.826	1.00	33.46	6
	ATOM	3578	O	LEU	B	184	72.300	-8.130	34.314	1.00	32.16	8
60	ATOM	3579	CB	LEU	B	184	74.325	-7.737	36.370	1.00	32.38	6
	ATOM	3580	CG	LEU	B	184	75.481	-7.019	35.655	1.00	32.34	6
	ATOM	3581	CD1	LEU	B	184	75.643	-5.559	36.125	1.00	34.61	6
	ATOM	3582	CD2	LEU	B	184	76.748	-7.838	35.853	1.00	34.57	6
	ATOM	3583	N	ALA	B	185	72.466	-5.818	34.204	1.00	32.96	7
65	ATOM	3584	CA	ALA	B	185	72.099	-5.821	32.780	1.00	33.17	6
	ATOM	3585	C	ALA	B	185	73.053	-6.670	31.950	1.00	35.69	6
	ATOM	3586	O	ALA	B	185	74.281	-6.510	32.057	1.00	35.57	8
	ATOM	3587	CB	ALA	B	185	72.076	-4.368	32.316	1.00	29.95	6
	ATOM	1443	N	LEU	B	186	72.752	-7.823	31.203	1.00	16.87	
70	ATOM	1444	CA	LEU	B	186	73.699	-8.676	30.476	1.00	16.99	
	ATOM	1445	C	LEU	B	186	74.354	-7.793	29.406	1.00	17.67	
	ATOM	1446	O	LEU	B	186	73.662	-7.050	28.666	1.00	20.34	
	ATOM	1447	CB	LEU	B	186	73.001	-9.890	29.872	1.00	16.87	
	ATOM	1448	CG	LEU	B	186	72.315	-10.841	30.851	1.00	18.67	
	ATOM	1449	CD1	LEU	B	186	71.803	-12.062	30.097	1.00	20.67	

-85-

	ATOM	1450	CD2	LEU	B	186	73.289	-11.257	31.936	1.00	17.31	
	ATOM	1451	N	SER	B	187	75.650	-7.991	29.285	1.00	18.83	
	ATOM	1452	CA	SER	B	187	76.407	-7.179	28.327	1.00	17.18	
5	ATOM	1453	C	SER	B	187	77.754	-7.771	28.079	1.00	17.64	
	ATOM	1454	O	SER	B	187	78.405	-8.305	28.987	1.00	18.63	
	ATOM	1455	CB	SER	B	187	76.597	-5.762	28.933	1.00	20.23	
	ATOM	1456	OG	SER	B	187	77.485	-4.989	28.093	1.00	20.91	
	ATOM	1457	N	SER	B	188	78.290	-7.564	26.832	1.00	17.55	
10	ATOM	1458	CA	SER	B	188	79.706	-7.917	26.649	1.00	17.70	
	ATOM	1459	C	SER	B	188	80.653	-7.182	27.579	1.00	17.74	
	ATOM	1460	O	SER	B	188	81.764	-7.648	27.944	1.00	18.92	
	ATOM	1461	CB	SER	B	188	80.127	-7.598	25.196	1.00	19.73	
	ATOM	1462	OG	SER	B	188	79.893	-6.208	24.915	1.00	20.84	
15	ATOM	1463	N	ARG	B	189	80.298	-6.012	28.096	1.00	18.16	
	ATOM	1464	CA	ARG	B	189	81.104	-5.205	28.988	1.00	19.85	
	ATOM	1465	C	ARG	B	189	81.386	-5.909	30.311	1.00	20.33	
	ATOM	1466	O	ARG	B	189	82.356	-5.612	30.969	1.00	21.91	
	ATOM	1467	CB	ARG	B	189	80.426	-3.848	29.284	1.00	20.55	
20	ATOM	1468	CG	ARG	B	189	80.245	-3.075	27.973	1.00	22.89	
	ATOM	1469	CD	ARG	B	189	79.609	-1.707	28.273	1.00	23.21	
	ATOM	1470	NE	ARG	B	189	79.461	-1.073	26.939	1.00	25.97	
	ATOM	1471	CZ	ARG	B	189	79.880	0.157	26.683	1.00	28.29	
	ATOM	1472	NH1	ARG	B	189	80.387	0.915	27.617	1.00	26.60	
25	ATOM	1473	NH2	ARG	B	189	79.714	0.627	25.429	1.00	28.41	
	ATOM	1474	N	ASN	B	190	80.441	-6.790	30.763	1.00	19.42	
	ATOM	1475	CA	ASN	B	190	80.639	-7.442	32.041	1.00	19.64	
	ATOM	1476	C	ASN	B	190	81.891	-8.271	32.059	1.00	22.61	
	ATOM	1477	O	ASN	B	190	82.467	-8.717	33.097	1.00	23.27	
30	ATOM	1478	CB	ASN	B	190	79.437	-8.347	32.355	1.00	19.54	
	ATOM	1479	CG	ASN	B	190	78.168	-7.518	32.494	1.00	21.41	
	ATOM	1480	OD1	ASN	B	190	77.045	-8.077	32.323	1.00	21.40	
	ATOM	1481	ND2	ASN	B	190	78.310	-6.244	32.814	1.00	19.16	
	ATOM	1497	N	GLY	B	191	82.333	-8.712	30.735	1.00	27.44	
35	ATOM	1498	CA	GLY	B	191	83.554	-9.514	30.632	1.00	28.04	
	ATOM	1499	C	GLY	B	191	84.823	-8.796	31.035	1.00	29.70	
	ATOM	1500	O	GLY	B	191	85.815	-9.487	31.266	1.00	31.47	
	ATOM	1482	N	TYR	B	192	84.825	-7.501	31.228	1.00	26.92	
	ATOM	1483	CA	TYR	B	192	86.032	-6.786	31.629	1.00	29.88	
40	ATOM	1484	C	TYR	B	192	86.054	-6.581	33.125	1.00	29.91	
	ATOM	1485	O	TYR	B	192	87.053	-5.998	33.601	1.00	34.28	
	ATOM	1486	CB	TYR	B	192	86.154	-5.424	30.922	1.00	30.32	
	ATOM	1487	CG	TYR	B	192	86.340	-5.687	29.438	1.00	32.17	
	ATOM	1488	CD1	TYR	B	192	85.211	-5.943	28.667	1.00	32.38	
45	ATOM	1489	CD2	TYR	B	192	87.596	-5.764	28.842	1.00	34.00	
	ATOM	1490	CE1	TYR	B	192	85.313	-6.234	27.337	1.00	35.21	
	ATOM	1491	CE2	TYR	B	192	87.703	-6.056	27.486	1.00	34.55	
	ATOM	1492	CZ	TYR	B	192	86.578	-6.276	26.747	1.00	36.66	
	ATOM	1493	OH	TYR	B	192	86.631	-6.577	25.395	1.00	38.33	
50	ATOM	1494	N	LEU	B	193	85.033	-7.028	33.865	1.00	28.20	
	ATOM	1495	CA	LEU	B	193	85.075	-6.900	35.299	1.00	26.63	
	ATOM	1496	C	LEU	B	193	85.870	-7.994	35.986	1.00	27.15	
	ATOM	1497	O	LEU	B	193	85.690	-9.155	35.614	1.00	28.28	
	ATOM	1498	CB	LEU	B	193	83.651	-6.979	35.888	1.00	26.20	
55	ATOM	1499	CG	LEU	B	193	82.648	-5.971	35.339	1.00	25.58	
	ATOM	1500	CD1	LEU	B	193	81.223	-6.375	35.649	1.00	24.08	
	ATOM	1501	CD2	LEU	B	193	82.909	-4.563	35.910	1.00	27.77	
	ATOM	1502	N	THR	B	194	86.596	-7.704	37.090	1.00	28.42	
	ATOM	1503	CA	THR	B	194	87.177	-8.819	37.838	1.00	27.62	
60	ATOM	1504	C	THR	B	194	86.087	-9.564	38.585	1.00	25.74	
	ATOM	1505	O	THR	B	194	84.983	-8.990	38.712	1.00	26.48	
	ATOM	1506	CB	THR	B	194	88.236	-8.313	38.835	1.00	29.34	
	ATOM	1507	OG1	THR	B	194	87.611	-7.354	39.693	1.00	30.55	
	ATOM	1508	CG2	THR	B	194	89.370	-7.647	38.064	1.00	32.65	
65	ATOM	3620	N	ALA	B	195	86.095	-11.397	38.739	1.00	45.01	7
	ATOM	3621	CA	ALA	B	195	85.137	-12.052	39.619	1.00	45.61	6
	ATOM	3622	C	ALA	B	195	84.702	-11.095	40.732	1.00	46.90	6
	ATOM	3623	O	ALA	B	195	83.510	-11.093	41.082	1.00	45.91	8
	ATOM	3624	CB	ALA	B	195	85.717	-13.336	40.196	1.00	46.79	6
	ATOM	3625	N	GLU	B	196	85.603	-10.280	41.278	1.00	47.33	7
70	ATOM	3626	CA	GLU	B	196	85.242	-9.350	42.330	1.00	48.34	6
	ATOM	3627	C	GLU	B	196	84.313	-8.252	41.828	1.00	46.99	6
	ATOM	3628	O	GLU	B	196	83.325	-7.912	42.497	1.00	47.72	8
	ATOM	3629	CB	GLU	B	196	86.459	-8.634	42.959	1.00	52.20	6
	ATOM	3630	CG	GLU	B	196	86.011	-7.646	44.018	1.00	56.19	6

-86-

	ATOM	3631	CD	GLU	B	196	86.989	-6.639	44.543	1.00	59.41	6
	ATOM	3632	OE1	GLU	B	196	88.104	-6.474	43.993	1.00	61.45	8
	ATOM	3633	OE2	GLU	B	196	86.639	-5.966	45.555	1.00	61.84	8
5	ATOM	3634	N	GLN	B	197	84.641	-7.664	40.687	1.00	44.75	7
	ATOM	3635	CA	GLN	B	197	83.801	-6.624	40.095	1.00	43.46	6
	ATOM	3636	C	GLN	B	197	82.428	-7.188	39.782	1.00	42.72	6
	ATOM	3637	O	GLN	B	197	81.425	-6.478	39.983	1.00	41.97	8
	ATOM	3638	CB	GLN	B	197	84.430	-6.018	38.832	1.00	43.86	6
10	ATOM	3639	CG	GLN	B	197	85.754	-5.346	39.203	1.00	46.24	6
	ATOM	3640	CD	GLN	B	197	86.485	-4.709	38.047	1.00	48.63	6
	ATOM	3641	OE1	GLN	B	197	86.387	-5.148	36.902	1.00	50.12	8
	ATOM	3642	NE2	GLN	B	197	87.247	-3.655	38.397	1.00	49.65	7
	ATOM	3643	N	ARG	B	198	82.339	-8.436	39.342	1.00	40.11	7
15	ATOM	3644	CA	ARG	B	198	81.024	-9.023	39.025	1.00	40.65	6
	ATOM	3645	C	ARG	B	198	80.231	-9.134	40.321	1.00	40.50	6
	ATOM	3646	O	ARG	B	198	79.001	-9.070	40.226	1.00	40.26	8
	ATOM	3647	CB	ARG	B	198	81.196	-10.331	38.255	1.00	38.75	6
	ATOM	3648	CG	ARG	B	198	79.950	-11.169	37.980	1.00	40.23	6
20	ATOM	3649	CD	ARG	B	198	78.984	-10.360	37.114	1.00	38.56	6
	ATOM	3650	NE	ARG	B	198	77.712	-10.999	36.860	1.00	40.33	7
	ATOM	3651	CZ	ARG	B	198	76.685	-10.913	37.703	1.00	38.73	6
	ATOM	3652	NH1	ARG	B	198	76.828	-10.212	38.843	1.00	37.38	7
	ATOM	3653	NH2	ARG	B	198	75.530	-11.506	37.383	1.00	39.11	7
25	ATOM	3654	N	LYS	B	199	80.821	-9.198	41.506	1.00	40.18	7
	ATOM	3655	CA	LYS	B	199	80.067	-9.237	42.738	1.00	41.84	6
	ATOM	3656	C	LYS	B	199	79.519	-7.843	43.083	1.00	39.14	6
	ATOM	3657	O	LYS	B	199	78.440	-7.806	43.660	1.00	39.85	8
	ATOM	3658	CB	LYS	B	199	80.852	-9.706	43.969	1.00	44.70	6
30	ATOM	3659	CG	LYS	B	199	81.675	-10.963	43.783	1.00	48.43	6
	ATOM	3660	CD	LYS	B	199	82.186	-11.540	45.087	1.00	50.67	6
	ATOM	3661	CE	LYS	B	199	82.837	-10.559	46.037	1.00	52.79	6
	ATOM	3662	NZ	LYS	B	199	84.285	-10.286	45.751	1.00	55.36	7
	ATOM	3663	N	ILE	B	200	80.245	-6.791	42.754	1.00	36.48	7
35	ATOM	3664	CA	ILE	B	200	79.815	-5.425	43.013	1.00	36.30	6
	ATOM	3665	C	ILE	B	200	78.867	-4.836	41.964	1.00	34.09	6
	ATOM	3666	O	ILE	B	200	77.970	-4.048	42.300	1.00	31.98	8
	ATOM	3667	CB	ILE	B	200	81.036	-4.477	43.052	1.00	37.30	6
	ATOM	3668	CG1	ILE	B	200	81.938	-4.835	44.261	1.00	39.39	6
40	ATOM	3669	CG2	ILE	B	200	80.668	-2.995	43.087	1.00	38.32	6
	ATOM	3670	CD1	ILE	B	200	83.228	-4.024	44.171	1.00	39.23	6
	ATOM	3671	N	ALA	B	201	78.923	-5.343	40.749	1.00	31.89	7
	ATOM	3672	CA	ALA	B	201	78.199	-4.790	39.605	1.00	30.33	6
	ATOM	3673	C	ALA	B	201	76.683	-4.738	39.757	1.00	30.26	6
45	ATOM	3674	O	ALA	B	201	76.126	-3.736	39.270	1.00	28.19	8
	ATOM	3675	CB	ALA	B	201	78.588	-5.549	38.327	1.00	31.33	6
	ATOM	3676	N	PRO	B	202	75.978	-5.632	40.395	1.00	29.89	7
	ATOM	3677	CA	PRO	B	202	74.538	-5.483	40.618	1.00	31.17	6
	ATOM	3678	C	PRO	B	202	74.130	-4.220	41.350	1.00	30.89	6
50	ATOM	3679	O	PRO	B	202	72.942	-3.842	41.356	1.00	33.70	8
	ATOM	3680	CB	PRO	B	202	74.171	-6.714	41.422	1.00	31.80	6
	ATOM	3681	CG	PRO	B	202	75.203	-7.727	41.041	1.00	32.51	6
	ATOM	3682	CD	PRO	B	202	76.485	-6.926	40.935	1.00	30.92	6
	ATOM	3683	N	GLY	B	203	75.003	-3.520	42.079	1.00	30.61	7
55	ATOM	3684	CA	GLY	B	203	74.724	-2.274	42.775	1.00	29.71	6
	ATOM	3685	C	GLY	B	203	74.185	-1.180	41.844	1.00	29.14	6
	ATOM	3686	O	GLY	B	203	73.382	-0.333	42.278	1.00	27.39	8
	ATOM	3687	N	LEU	B	204	74.569	-1.208	40.562	1.00	26.29	7
	ATOM	3688	CA	LEU	B	204	74.116	-0.193	39.634	1.00	27.87	6
60	ATOM	3689	C	LEU	B	204	72.595	-0.279	39.482	1.00	26.50	6
	ATOM	3690	O	LEU	B	204	71.878	0.736	39.532	1.00	26.32	8
	ATOM	3691	CB	LEU	B	204	74.789	-0.294	38.259	1.00	28.45	6
	ATOM	3692	CG	LEU	B	204	74.362	0.731	37.212	1.00	29.87	6
	ATOM	3693	CD1	LEU	B	204	74.600	2.168	37.697	1.00	31.40	6
65	ATOM	3694	CD2	LEU	B	204	75.087	0.559	35.887	1.00	32.44	6
	ATOM	3695	N	TYR	B	205	72.132	-1.509	39.245	1.00	26.81	7
	ATOM	3696	CA	TYR	B	205	70.667	-1.619	39.081	1.00	28.26	6
	ATOM	3697	C	TYR	B	205	69.946	-1.322	40.382	1.00	28.28	6
	ATOM	3698	O	TYR	B	205	68.816	-0.829	40.340	1.00	27.87	8
70	ATOM	3699	CB	TYR	B	205	70.328	-2.995	38.524	1.00	27.88	6
	ATOM	3700	CG	TYR	B	205	68.848	-3.144	38.265	1.00	30.23	6
	ATOM	3701	CD1	TYR	B	205	68.193	-2.323	37.360	1.00	30.41	6
	ATOM	3702	CD2	TYR	B	205	68.111	-4.106	38.935	1.00	32.30	6
	ATOM	3703	CE1	TYR	B	205	66.838	-2.493	37.115	1.00	31.17	6
	ATOM	3704	CE2	TYR	B	205	66.743	-4.304	38.698	1.00	32.16	6

-87-

	ATOM	3705	CZ	TYR	B	205	66.134	-3.480	37.784	1.00	33.79	6
	ATOM	3706	OH	TYR	B	205	64.774	-3.587	37.529	1.00	36.69	8
	ATOM	3707	N	LYS	B	206	70.554	-1.567	41.568	1.00	27.79	7
	ATOM	3708	CA	LYS	B	206	69.949	-1.137	42.812	1.00	28.48	6
5	ATOM	3709	C	LYS	B	206	69.794	0.379	42.849	1.00	26.89	6
	ATOM	3710	O	LYS	B	206	68.729	0.847	43.295	1.00	26.06	8
	ATOM	3711	CB	LYS	B	206	70.814	-1.650	44.005	1.00	31.12	6
	ATOM	3712	CG	LYS	B	206	70.702	-3.191	44.056	1.00	35.12	6
10	ATOM	3713	CD	LYS	B	206	71.439	-3.803	45.235	1.00	38.80	6
	ATOM	3714	CE	LYS	B	206	71.267	-5.329	45.230	1.00	41.11	6
	ATOM	3715	NZ	LYS	B	206	72.055	-5.939	46.361	1.00	44.45	7
	ATOM	3716	N	VAL	B	207	70.786	1.151	42.450	1.00	24.10	7
	ATOM	3717	CA	VAL	B	207	70.698	2.623	42.437	1.00	23.57	6
15	ATOM	3718	C	VAL	B	207	69.692	3.075	41.353	1.00	25.00	6
	ATOM	3719	O	VAL	B	207	68.785	3.854	41.709	1.00	25.30	8
	ATOM	3720	CB	VAL	B	207	72.075	3.263	42.273	1.00	25.80	6
	ATOM	3721	CG1	VAL	B	207	71.998	4.765	42.088	1.00	24.61	6
	ATOM	3722	CG2	VAL	B	207	72.941	2.900	43.507	1.00	26.07	6
20	ATOM	3723	N	LEU	B	208	69.679	2.455	40.200	1.00	25.37	7
	ATOM	3724	CA	LEU	B	208	68.640	2.782	39.185	1.00	25.10	6
	ATOM	3725	C	LEU	B	208	67.243	2.553	39.694	1.00	24.92	6
	ATOM	3726	O	LEU	B	208	66.280	3.338	39.468	1.00	25.42	8
	ATOM	3727	CB	LEU	B	208	68.989	1.910	37.985	1.00	26.66	6
25	ATOM	3728	CG	LEU	B	208	68.261	2.079	36.661	1.00	30.34	6
	ATOM	3729	CD1	LEU	B	208	68.389	3.525	36.163	1.00	32.04	6
	ATOM	3730	CD2	LEU	B	208	68.793	1.084	35.646	1.00	31.70	6
	ATOM	3731	N	SER	B	209	67.019	1.416	40.355	1.00	26.22	7
30	ATOM	3732	CA	SER	B	209	65.726	1.035	40.907	1.00	29.64	6
	ATOM	3733	C	SER	B	209	65.293	2.025	41.988	1.00	30.28	6
	ATOM	3734	O	SER	B	209	64.107	2.380	42.055	1.00	30.20	8
	ATOM	3735	CB	SER	B	209	65.710	-0.386	41.480	1.00	30.00	6
	ATOM	3736	OG	SER	B	209	65.923	-1.312	40.425	1.00	32.79	8
	ATOM	3737	N	SER	B	210	66.262	2.526	42.772	1.00	29.87	7
35	ATOM	3738	CA	SER	B	210	65.938	3.533	43.764	1.00	30.73	6
	ATOM	3739	C	SER	B	210	65.469	4.839	43.141	1.00	28.63	6
	ATOM	3740	O	SER	B	210	64.551	5.481	43.694	1.00	30.02	8
	ATOM	3741	CB	SER	B	210	67.171	3.837	44.652	1.00	33.65	6
	ATOM	3742	OG	SER	B	210	66.847	4.965	45.451	1.00	38.88	8
40	ATOM	3743	N	ILE	B	211	66.115	5.259	42.067	1.00	26.67	7
	ATOM	3744	CA	ILE	B	211	65.727	6.462	41.337	1.00	26.97	6
	ATOM	3745	C	ILE	B	211	64.283	6.278	40.860	1.00	29.84	6
	ATOM	3746	O	ILE	B	211	63.426	7.151	41.011	1.00	29.98	8
	ATOM	3747	CB	ILE	B	211	66.584	6.759	40.124	1.00	26.70	6
45	ATOM	3748	CG1	ILE	B	211	68.031	7.036	40.607	1.00	26.03	6
	ATOM	3749	CG2	ILE	B	211	66.046	7.935	39.290	1.00	27.20	6
	ATOM	3750	CD1	ILE	B	211	69.081	7.179	39.551	1.00	25.43	6
	ATOM	3751	N	ALA	B	212	64.062	5.111	40.250	1.00	29.63	7
50	ATOM	3752	CA	ALA	B	212	62.703	4.840	39.732	1.00	31.76	6
	ATOM	3753	C	ALA	B	212	61.680	4.874	40.827	1.00	33.70	6
	ATOM	3754	O	ALA	B	212	60.601	5.488	40.669	1.00	35.70	8
	ATOM	3755	CB	ALA	B	212	62.713	3.477	39.041	1.00	30.18	6
	ATOM	3756	N	ASP	B	213	61.985	4.267	41.976	1.00	35.57	7
	ATOM	3757	CA	ASP	B	213	61.051	4.267	43.097	1.00	37.44	6
55	ATOM	3758	C	ASP	B	213	60.766	5.705	43.541	1.00	38.51	6
	ATOM	3759	O	ASP	B	213	59.588	5.981	43.821	1.00	39.54	8
	ATOM	3760	CB	ASP	B	213	61.540	3.469	44.294	1.00	40.83	6
	ATOM	3761	CG	ASP	B	213	61.594	1.978	44.075	1.00	43.42	6
	ATOM	3762	OD1	ASP	B	213	60.952	1.468	43.127	1.00	44.23	8
60	ATOM	3763	OD2	ASP	B	213	62.266	1.294	44.889	1.00	45.13	8
	ATOM	3764	N	LYS	B	214	61.739	6.605	43.622	1.00	36.89	7
	ATOM	3765	CA	LYS	B	214	61.439	7.980	44.023	1.00	37.14	6
	ATOM	3766	C	LYS	B	214	60.553	8.695	43.015	1.00	38.10	6
	ATOM	3767	O	LYS	B	214	59.689	9.521	43.354	1.00	38.08	8
65	ATOM	3768	CB	LYS	B	214	62.734	8.783	44.210	1.00	35.35	6
	ATOM	3769	CG	LYS	B	214	63.592	8.274	45.353	1.00	34.18	6
	ATOM	3770	CD	LYS	B	214	64.924	9.016	45.447	1.00	33.76	6
	ATOM	3771	CE	LYS	B	214	65.708	8.660	46.703	1.00	35.46	6
	ATOM	3772	NZ	LYS	B	214	66.968	9.471	46.836	1.00	33.81	7
70	ATOM	3773	N	LEU	B	215	60.824	8.468	41.720	1.00	37.41	7
	ATOM	3774	CA	LEU	B	215	60.005	9.116	40.679	1.00	38.52	6
	ATOM	3775	C	LEU	B	215	58.575	8.587	40.776	1.00	41.72	6
	ATOM	3776	O	LEU	B	215	57.606	9.372	40.631	1.00	41.98	8
	ATOM	3777	CB	LEU	B	215	60.604	8.904	39.310	1.00	37.43	6
	ATOM	3778	CG	LEU	B	215	61.897	9.594	38.900	1.00	36.45	6

-88-

	ATOM	3779	CD1	LEU	B	215	62.313	9.105	37.529	1.00	36.60	6
	ATOM	3780	CD2	LEU	B	215	61.767	11.119	38.869	1.00	37.66	6
	ATOM	3781	N	GLN	B	216	58.409	7.300	41.061	1.00	42.52	7
5	ATOM	3782	CA	GLN	B	216	57.077	6.739	41.231	1.00	46.61	6
	ATOM	3783	C	GLN	B	216	56.353	7.337	42.439	1.00	47.19	6
	ATOM	3784	O	GLN	B	216	55.125	7.438	42.427	1.00	48.78	8
	ATOM	3785	CB	GLN	B	216	57.069	5.232	41.449	1.00	48.29	6
	ATOM	3786	CG	GLN	B	216	57.290	4.444	40.180	1.00	53.02	6
	ATOM	3787	CD	GLN	B	216	56.839	3.002	40.322	1.00	54.94	6
10	ATOM	3788	OE1	GLN	B	216	55.736	2.658	39.896	1.00	57.54	8
	ATOM	3789	NE2	GLN	B	216	57.710	2.210	40.927	1.00	55.50	7
	ATOM	3790	N	ALA	B	217	57.092	7.678	43.486	1.00	46.68	7
	ATOM	3791	CA	ALA	B	217	56.502	8.282	44.665	1.00	47.12	6
	ATOM	3792	C	ALA	B	217	56.114	9.746	44.444	1.00	46.63	6
15	ATOM	3793	O	ALA	B	217	55.403	10.274	45.308	1.00	47.81	8
	ATOM	3794	CB	ALA	B	217	57.460	8.177	45.853	1.00	46.15	6
	ATOM	3795	N	GLY	B	218	56.519	10.406	43.374	1.00	45.52	7
	ATOM	3796	CA	GLY	B	218	56.156	11.790	43.127	1.00	45.00	6
	ATOM	3797	C	GLY	B	218	57.308	12.764	43.230	1.00	45.03	6
20	ATOM	3798	O	GLY	B	218	57.199	13.970	42.964	1.00	45.86	8
	ATOM	3799	N	GLU	B	219	58.491	12.255	43.605	1.00	43.84	7
	ATOM	3800	CA	GLU	B	219	59.664	13.121	43.708	1.00	43.09	6
	ATOM	3801	C	GLU	B	219	60.052	13.746	42.388	1.00	40.95	6
	ATOM	3802	O	GLU	B	219	60.141	13.088	41.333	1.00	39.42	8
25	ATOM	3803	CB	GLU	B	219	60.804	12.270	44.287	1.00	45.88	6
	ATOM	3804	CG	GLU	B	219	61.238	12.787	45.633	1.00	50.50	6
	ATOM	3805	CD	GLU	B	219	62.401	12.048	46.269	1.00	52.33	6
	ATOM	3806	OE1	GLU	B	219	62.065	11.125	47.052	1.00	54.16	8
	ATOM	3807	OE2	GLU	B	219	63.564	12.388	46.016	1.00	53.19	8
30	ATOM	3808	N	ARG	B	220	60.247	15.065	42.373	1.00	38.26	7
	ATOM	3809	CA	ARG	B	220	60.572	15.785	41.151	1.00	38.87	6
	ATOM	3810	C	ARG	B	220	61.803	16.664	41.272	1.00	38.94	6
	ATOM	3811	O	ARG	B	220	62.119	17.358	40.305	1.00	39.85	8
35	ATOM	3812	CB	ARG	B	220	59.396	16.676	40.670	1.00	39.03	6
	ATOM	3813	CG	ARG	B	220	58.187	15.871	40.179	1.00	39.62	6
	ATOM	3814	CD	ARG	B	220	58.562	15.016	38.972	1.00	39.07	6
	ATOM	3815	NE	ARG	B	220	57.490	14.110	38.632	1.00	39.25	7
	ATOM	3816	CZ	ARG	B	220	57.184	12.886	39.019	1.00	39.75	6
	ATOM	3817	NH1	ARG	B	220	57.946	12.211	39.893	1.00	39.07	7
40	ATOM	3818	NH2	ARG	B	220	56.073	12.331	38.529	1.00	38.25	7
	ATOM	3819	N	ASP	B	221	62.564	16.577	42.361	1.00	38.00	7
	ATOM	3820	CA	ASP	B	221	63.792	17.372	42.433	1.00	38.21	6
	ATOM	3821	C	ASP	B	221	64.911	16.557	41.791	1.00	36.88	6
	ATOM	3822	O	ASP	B	221	65.691	15.899	42.474	1.00	36.84	8
45	ATOM	3823	CB	ASP	B	221	64.146	17.760	43.866	1.00	40.08	6
	ATOM	3824	CG	ASP	B	221	65.276	18.775	43.867	1.00	40.98	6
	ATOM	3825	OD1	ASP	B	221	66.189	18.865	43.017	1.00	40.33	8
	ATOM	3826	OD2	ASP	B	221	65.237	19.583	44.824	1.00	45.27	8
50	ATOM	3827	N	LEU	B	222	64.940	16.559	40.472	1.00	36.51	7
	ATOM	3828	CA	LEU	B	222	65.839	15.703	39.697	1.00	35.37	6
	ATOM	3829	C	LEU	B	222	67.312	15.852	40.004	1.00	34.02	6
	ATOM	3830	O	LEU	B	222	68.053	14.855	40.041	1.00	31.24	8
	ATOM	3831	CB	LEU	B	222	65.575	15.983	38.203	1.00	35.83	6
55	ATOM	3832	CG	LEU	B	222	64.144	15.686	37.720	1.00	38.11	6
	ATOM	3833	CD1	LEU	B	222	64.187	15.314	36.239	1.00	38.86	6
	ATOM	3834	CD2	LEU	B	222	63.430	14.608	38.526	1.00	36.91	6
	ATOM	3835	N	ASP	B	223	67.763	17.101	40.153	1.00	33.49	7
	ATOM	3836	CA	ASP	B	223	69.154	17.349	40.442	1.00	33.63	6
	ATOM	3837	C	ASP	B	223	69.524	16.656	41.751	1.00	31.73	6
60	ATOM	3838	O	ASP	B	223	70.620	16.132	41.870	1.00	31.34	8
	ATOM	3839	CB	ASP	B	223	69.494	18.827	40.653	1.00	34.33	6
	ATOM	3840	N	GLU	B	224	68.635	16.790	42.733	1.00	31.71	7
	ATOM	3841	CA	GLU	B	224	68.909	16.161	44.035	1.00	31.51	6
	ATOM	3842	C	GLU	B	224	68.836	14.656	43.974	1.00	29.02	6
65	ATOM	3843	O	GLU	B	224	69.667	13.945	44.502	1.00	28.00	8
	ATOM	3844	CB	GLU	B	224	67.907	16.696	45.089	1.00	34.56	6
	ATOM	3845	CG	GLU	B	224	68.123	16.063	46.454	1.00	37.72	6
	ATOM	3846	CD	GLU	B	224	69.389	16.542	47.140	1.00	42.79	6
	ATOM	3847	OE1	GLU	B	224	70.120	17.403	46.574	1.00	43.28	8
70	ATOM	3848	OE2	GLU	B	224	69.660	16.051	48.273	1.00	43.45	8
	ATOM	3849	N	ILE	B	225	67.863	14.079	43.231	1.00	27.24	7
	ATOM	3850	CA	ILE	B	225	67.835	12.642	43.056	1.00	26.19	6
	ATOM	3851	C	ILE	B	225	69.109	12.145	42.417	1.00	25.15	6
	ATOM	3852	O	ILE	B	225	69.651	11.121	42.828	1.00	26.25	8

-89-

	ATOM	3853	CB	ILE	B	225	66.632	12.214	42.152	1.00	28.29	6
	ATOM	3854	CG1	ILE	B	225	65.340	12.494	42.878	1.00	29.03	6
	ATOM	3855	CG2	ILE	B	225	66.803	10.740	41.776	1.00	25.65	6
5	ATOM	3856	CD1	ILE	B	225	64.109	12.596	42.001	1.00	31.93	6
	ATOM	3857	N	ILE	B	226	69.578	12.801	41.373	1.00	26.43	7
	ATOM	3858	CA	ILE	B	226	70.786	12.406	40.641	1.00	25.84	6
	ATOM	3859	C	ILE	B	226	72.040	12.551	41.500	1.00	27.10	6
	ATOM	3860	O	ILE	B	226	72.923	11.716	41.451	1.00	24.94	8
10	ATOM	3861	CB	ILE	B	226	70.923	13.170	39.304	1.00	27.17	6
	ATOM	3862	CG1	ILE	B	226	69.753	12.662	38.429	1.00	27.18	6
	ATOM	3863	CG2	ILE	B	226	72.280	12.981	38.632	1.00	27.48	6
	ATOM	3864	CD1	ILE	B	226	69.562	13.504	37.159	1.00	27.31	6
	ATOM	3865	N	THR	B	227	72.095	13.642	42.283	1.00	25.81	7
15	ATOM	3866	CA	THR	B	227	73.300	13.811	43.112	1.00	25.80	6
	ATOM	3867	C	THR	B	227	73.368	12.725	44.157	1.00	24.81	6
	ATOM	3868	O	THR	B	227	74.457	12.188	44.484	1.00	23.72	8
	ATOM	3869	CB	THR	B	227	73.230	15.226	43.714	1.00	25.87	6
	ATOM	3870	OG1	THR	B	227	73.461	16.226	42.719	1.00	27.10	8
20	ATOM	3871	CG2	THR	B	227	74.317	15.419	44.776	1.00	30.13	6
	ATOM	3872	N	ILE	B	228	72.202	12.447	44.753	1.00	21.50	7
	ATOM	3873	CA	ILE	B	228	72.230	11.384	45.756	1.00	21.63	6
	ATOM	3874	C	ILE	B	228	72.645	10.046	45.160	1.00	23.87	6
	ATOM	3875	O	ILE	B	228	73.410	9.242	45.679	1.00	22.19	8
25	ATOM	3876	CB	ILE	B	228	70.892	11.236	46.481	1.00	21.84	6
	ATOM	3877	CG1	ILE	B	228	70.746	12.501	47.397	1.00	24.08	6
	ATOM	3878	CG2	ILE	B	228	70.762	9.964	47.278	1.00	22.76	6
	ATOM	3879	CD1	ILE	B	228	69.295	12.583	47.901	1.00	26.19	6
	ATOM	3880	N	ALA	B	229	72.035	9.747	43.962	1.00	23.45	7
30	ATOM	3881	CA	ALA	B	229	72.386	8.510	43.308	1.00	24.32	6
	ATOM	3882	C	ALA	B	229	73.835	8.419	42.943	1.00	21.10	6
	ATOM	3883	O	ALA	B	229	74.403	7.325	43.107	1.00	23.01	8
	ATOM	3884	CB	ALA	B	229	71.481	8.404	42.050	1.00	22.78	6
	ATOM	3885	N	GLY	B	230	74.533	9.496	42.596	1.00	22.98	7
35	ATOM	3886	CA	GLY	B	230	75.940	9.540	42.325	1.00	25.69	6
	ATOM	3887	C	GLY	B	230	76.731	9.266	43.636	1.00	25.98	6
	ATOM	3888	O	GLY	B	230	77.669	8.455	43.656	1.00	23.67	8
	ATOM	3889	N	GLN	B	231	76.233	9.789	44.748	1.00	25.92	7
	ATOM	3890	CA	GLN	B	231	76.907	9.478	46.035	1.00	27.99	6
40	ATOM	3891	C	GLN	B	231	76.700	8.048	46.427	1.00	26.47	6
	ATOM	3892	O	GLN	B	231	77.666	7.384	46.850	1.00	25.84	8
	ATOM	3893	CB	GLN	B	231	76.407	10.471	47.120	1.00	28.03	6
	ATOM	3894	CG	GLN	B	231	76.834	10.043	48.531	1.00	32.38	6
	ATOM	3895	CD	GLN	B	231	78.316	10.219	48.756	1.00	32.95	6
45	ATOM	3896	OE1	GLN	B	231	79.045	10.701	47.905	1.00	33.95	8
	ATOM	3897	NE2	GLN	B	231	78.780	9.786	49.922	1.00	36.62	7
	ATOM	3898	N	GLU	B	232	75.516	7.434	46.178	1.00	26.86	7
	ATOM	3899	CA	GLU	B	232	75.285	6.024	46.475	1.00	25.40	6
	ATOM	3900	C	GLU	B	232	76.193	5.139	45.605	1.00	27.57	6
50	ATOM	3901	O	GLU	B	232	76.802	4.178	46.110	1.00	28.11	8
	ATOM	3902	CB	GLU	B	232	73.827	5.559	46.287	1.00	27.07	6
	ATOM	3903	CG	GLU	B	232	72.820	6.282	47.171	1.00	30.63	6
	ATOM	3904	CD	GLU	B	232	71.375	5.946	46.930	1.00	34.51	6
	ATOM	3905	OE1	GLU	B	232	71.033	5.379	45.860	1.00	37.23	8
55	ATOM	3906	OE2	GLU	B	232	70.510	6.232	47.794	1.00	35.98	8
	ATOM	3907	N	LEU	B	233	76.346	5.489	44.313	1.00	26.60	7
	ATOM	3908	CA	LEU	B	233	77.272	4.700	43.490	1.00	26.30	6
	ATOM	3909	C	LEU	B	233	78.710	4.784	44.024	1.00	28.83	6
	ATOM	3910	O	LEU	B	233	79.402	3.781	44.040	1.00	28.19	8
60	ATOM	3911	CB	LEU	B	233	77.171	5.171	42.025	1.00	27.72	6
	ATOM	3912	CG	LEU	B	233	75.816	4.809	41.372	1.00	26.70	6
	ATOM	3913	CD1	LEU	B	233	75.511	5.576	40.104	1.00	27.51	6
	ATOM	3914	CD2	LEU	B	233	75.819	3.312	41.048	1.00	28.08	6
	ATOM	3915	N	ASN	B	234	79.166	6.006	44.330	1.00	31.21	7
65	ATOM	3916	CA	ASN	B	234	80.540	6.248	44.790	1.00	32.86	6
	ATOM	3917	C	ASN	B	234	80.761	5.404	46.020	1.00	32.80	6
	ATOM	3918	O	ASN	B	234	81.764	4.675	46.099	1.00	34.18	8
	ATOM	3919	CB	ASN	B	234	80.775	7.750	45.048	1.00	33.46	6
	ATOM	3920	CG	ASN	B	234	82.187	8.099	45.503	1.00	38.46	6
	ATOM	3921	OD1	ASN	B	234	82.545	7.889	46.687	1.00	39.27	8
70	ATOM	3922	ND2	ASN	B	234	83.042	8.646	44.636	1.00	38.37	7
	ATOM	3923	N	GLU	B	235	79.781	5.385	46.942	1.00	32.30	7
	ATOM	3924	CA	GLU	B	235	79.995	4.556	48.156	1.00	34.69	6
	ATOM	3925	C	GLU	B	235	80.036	3.082	47.880	1.00	35.00	6
	ATOM	3926	O	GLU	B	235	80.783	2.325	48.548	1.00	34.91	8

-90-

	ATOM	3927	CB	GLU	B	235	78.927	4.941	49.210	1.00	35.01	6
	ATOM	3928	N	LYS	B	236	79.431	2.541	46.819	1.00	32.85	7
	ATOM	3929	CA	LYS	B	236	79.476	1.161	46.438	1.00	32.12	6
5	ATOM	3930	C	LYS	B	236	80.733	0.795	45.662	1.00	31.23	6
	ATOM	3931	O	LYS	B	236	81.027	-0.387	45.442	1.00	32.24	8
	ATOM	3932	CB	LYS	B	236	78.257	0.838	45.530	1.00	31.56	6
	ATOM	3933	CG	LYS	B	236	76.968	0.739	46.321	1.00	33.04	6
	ATOM	3934	CD	LYS	B	236	75.825	0.425	45.347	1.00	34.58	6
10	ATOM	3935	CE	LYS	B	236	74.486	0.657	46.017	1.00	38.11	6
	ATOM	3936	NZ	LYS	B	236	74.152	-0.406	47.008	1.00	41.00	7
	ATOM	3937	N	GLY	B	237	81.463	1.790	45.196	1.00	31.15	7
	ATOM	3938	CA	GLY	B	237	82.701	1.595	44.467	1.00	32.69	6
	ATOM	3939	C	GLY	B	237	82.728	2.025	43.030	1.00	33.87	6
15	ATOM	3940	O	GLY	B	237	83.730	1.798	42.345	1.00	36.00	8
	ATOM	3941	N	PHE	B	238	81.635	2.625	42.522	1.00	30.77	7
	ATOM	3942	CA	PHE	B	238	81.579	3.079	41.154	1.00	31.26	6
	ATOM	3943	C	PHE	B	238	82.111	4.488	41.041	1.00	32.04	6
	ATOM	3944	O	PHE	B	238	82.216	5.186	42.067	1.00	32.73	8
20	ATOM	3945	CB	PHE	B	238	80.125	3.016	40.628	1.00	31.33	6
	ATOM	3946	CG	PHE	B	238	79.481	1.668	40.628	1.00	29.12	6
	ATOM	3947	CD1	PHE	B	238	78.935	1.079	41.736	1.00	29.70	6
	ATOM	3948	CD2	PHE	B	238	79.401	0.975	39.390	1.00	29.67	6
	ATOM	3949	CE1	PHE	B	238	78.325	-0.181	41.661	1.00	30.02	6
25	ATOM	3950	CE2	PHE	B	238	78.805	-0.265	39.328	1.00	28.39	6
	ATOM	3951	CZ	PHE	B	238	78.268	-0.858	40.457	1.00	29.71	6
	ATOM	3952	N	ARG	B	239	82.539	4.918	39.876	1.00	32.94	7
	ATOM	3953	CA	ARG	B	239	83.050	6.269	39.716	1.00	35.90	6
	ATOM	3954	C	ARG	B	239	82.426	6.906	38.487	1.00	38.53	6
30	ATOM	3955	O	ARG	B	239	81.735	6.244	37.694	1.00	38.62	8
	ATOM	3956	CB	ARG	B	239	84.581	6.280	39.597	1.00	35.70	6
	ATOM	3957	CG	ARG	B	239	85.340	5.894	40.856	1.00	36.08	6
	ATOM	3958	CD	ARG	B	239	85.108	6.926	41.956	1.00	35.58	6
	ATOM	3959	NE	ARG	B	239	85.710	6.612	43.215	1.00	36.21	7
35	ATOM	3960	CZ	ARG	B	239	85.280	5.815	44.190	1.00	37.41	6
	ATOM	3961	NH1	ARG	B	239	84.113	5.159	44.129	1.00	35.39	7
	ATOM	3962	NH2	ARG	B	239	86.015	5.707	45.288	1.00	35.70	7
	ATOM	3963	N	ALA	B	240	82.667	8.199	38.339	1.00	38.40	7
	ATOM	3964	CA	ALA	B	240	82.310	8.977	37.152	1.00	39.45	6
40	ATOM	3965	C	ALA	B	240	80.954	8.630	36.553	1.00	39.96	6
	ATOM	3966	O	ALA	B	240	80.846	8.388	35.348	1.00	41.59	8
	ATOM	3967	CB	ALA	B	240	83.408	8.761	36.103	1.00	39.64	6
	ATOM	3968	N	ASP	B	241	79.899	8.687	37.369	1.00	39.86	7
	ATOM	3969	CA	ASP	B	241	78.567	8.382	36.881	1.00	37.91	6
45	ATOM	3970	C	ASP	B	241	78.087	9.495	35.947	1.00	39.44	6
	ATOM	3971	O	ASP	B	241	78.464	10.658	36.063	1.00	38.78	8
	ATOM	3972	CB	ASP	B	241	77.554	8.232	38.028	1.00	39.68	6
	ATOM	3973	CG	ASP	B	241	77.464	9.573	38.758	1.00	42.34	6
	ATOM	3974	OD1	ASP	B	241	76.577	10.419	38.447	1.00	44.14	8
50	ATOM	3975	OD2	ASP	B	241	78.353	9.828	39.610	1.00	41.04	8
	ATOM	3976	N	ASP	B	242	77.220	9.122	35.028	1.00	36.17	7
	ATOM	3977	CA	ASP	B	242	76.543	10.050	34.122	1.00	36.78	6
	ATOM	3978	C	ASP	B	242	75.102	9.548	34.108	1.00	32.97	6
	ATOM	3979	O	ASP	B	242	74.890	8.412	33.654	1.00	32.78	8
55	ATOM	3980	CB	ASP	B	242	77.160	10.107	32.755	1.00	41.35	6
	ATOM	3981	CG	ASP	B	242	76.317	10.792	31.704	1.00	46.81	6
	ATOM	3982	OD1	ASP	B	242	76.414	10.318	30.543	1.00	50.98	8
	ATOM	3983	OD2	ASP	B	242	75.539	11.741	31.944	1.00	49.34	8
	ATOM	3984	N	ILE	B	243	74.204	10.301	34.710	1.00	29.36	7
60	ATOM	3985	CA	ILE	B	243	72.817	9.893	34.861	1.00	27.87	6
	ATOM	3986	C	ILE	B	243	71.890	10.907	34.213	1.00	28.93	6
	ATOM	3987	O	ILE	B	243	71.986	12.098	34.489	1.00	28.18	8
	ATOM	3988	CB	ILE	B	243	72.407	9.746	36.339	1.00	28.09	6
	ATOM	3989	CG1	ILE	B	243	73.240	8.680	37.065	1.00	28.98	6
65	ATOM	3990	CG2	ILE	B	243	70.934	9.373	36.477	1.00	26.56	6
	ATOM	3991	CD1	ILE	B	243	73.044	8.655	38.575	1.00	28.71	6
	ATOM	3992	N	GLN	B	244	70.912	10.442	33.437	1.00	27.35	7
	ATOM	3993	CA	GLN	B	244	69.944	11.390	32.837	1.00	29.56	6
	ATOM	3994	C	GLN	B	244	68.550	10.906	33.126	1.00	28.63	6
70	ATOM	3995	O	GLN	B	244	68.328	9.670	33.170	1.00	28.44	8
	ATOM	3996	CB	GLN	B	244	70.154	11.546	31.342	1.00	32.37	6
	ATOM	3997	CG	GLN	B	244	71.494	11.871	30.754	1.00	33.10	6
	ATOM	3998	N	ILE	B	245	67.580	11.792	33.287	1.00	28.47	7
	ATOM	3999	CA	ILE	B	245	66.194	11.454	33.560	1.00	27.98	6
	ATOM	4000	C	ILE	B	245	65.367	12.295	32.544	1.00	29.53	6

	ATOM	4001	O	ILE	B	245	65.647	13.473	32.427	1.00	28.72	8
	ATOM	4002	CB	ILE	B	245	65.647	11.723	34.955	1.00	30.08	6
	ATOM	4003	CG1	ILE	B	245	66.275	10.837	36.048	1.00	31.65	6
5	ATOM	4004	CG2	ILE	B	245	64.136	11.475	34.988	1.00	30.80	6
	ATOM	4005	CD1	ILE	B	245	65.994	11.415	37.433	1.00	33.41	6
	ATOM	4006	N	ARG	B	246	64.608	11.578	31.703	1.00	28.63	7
	ATOM	4007	CA	ARG	B	246	63.903	12.319	30.635	1.00	29.40	6
	ATOM	4008	C	ARG	B	246	62.475	11.841	30.597	1.00	29.33	6
	ATOM	4009	O	ARG	B	246	62.198	10.775	31.136	1.00	29.29	8
10	ATOM	4010	CB	ARG	B	246	64.481	12.084	29.252	1.00	33.51	6
	ATOM	4011	CG	ARG	B	246	65.896	12.479	29.026	1.00	37.29	6
	ATOM	4012	CD	ARG	B	246	66.517	12.212	27.672	1.00	42.16	6
	ATOM	4013	NE	ARG	B	246	67.527	13.251	27.472	1.00	47.11	7
	ATOM	4014	CZ	ARG	B	246	68.770	13.142	27.056	1.00	50.44	6
15	ATOM	4015	NH1	ARG	B	246	69.318	11.970	26.737	1.00	53.10	7
	ATOM	4016	NH2	ARG	B	246	69.502	14.252	26.974	1.00	51.57	7
	ATOM	4017	N	ASP	B	247	61.544	12.634	30.039	1.00	28.70	7
	ATOM	4018	CA	ASP	B	247	60.185	12.189	29.792	1.00	29.87	6
20	ATOM	4019	C	ASP	B	247	60.289	11.146	28.656	1.00	25.96	6
	ATOM	4020	O	ASP	B	247	60.989	11.431	27.671	1.00	27.47	8
	ATOM	4021	CB	ASP	B	247	59.303	13.349	29.389	1.00	31.15	6
	ATOM	4022	CG	ASP	B	247	57.894	13.014	28.997	1.00	33.47	6
	ATOM	4023	OD1	ASP	B	247	57.667	12.084	28.184	1.00	32.45	8
25	ATOM	4024	OD2	ASP	B	247	56.982	13.703	29.524	1.00	33.36	8
	ATOM	4025	N	ALA	B	248	59.759	9.981	28.873	1.00	27.20	7
	ATOM	4026	CA	ALA	B	248	59.987	8.893	27.906	1.00	28.58	6
	ATOM	4027	C	ALA	B	248	59.141	9.055	26.643	1.00	29.88	6
	ATOM	4028	O	ALA	B	248	59.444	8.315	25.702	1.00	29.99	8
30	ATOM	4029	CB	ALA	B	248	59.652	7.572	28.566	1.00	28.03	6
	ATOM	4030	N	ASP	B	249	58.121	9.877	26.724	1.00	28.08	7
	ATOM	4031	CA	ASP	B	249	57.293	10.116	25.513	1.00	30.80	6
	ATOM	4032	C	ASP	B	249	57.764	11.262	24.667	1.00	29.85	6
	ATOM	4033	O	ASP	B	249	57.690	11.217	23.402	1.00	30.23	8
35	ATOM	4034	CB	ASP	B	249	55.853	10.392	25.955	1.00	32.78	6
	ATOM	4035	CG	ASP	B	249	55.226	9.204	26.623	1.00	37.46	6
	ATOM	4036	OD1	ASP	B	249	55.538	8.084	26.164	1.00	39.14	8
	ATOM	4037	OD2	ASP	B	249	54.448	9.329	27.595	1.00	39.72	8
	ATOM	4038	N	THR	B	250	58.264	12.361	25.283	1.00	26.32	7
40	ATOM	4039	CA	THR	B	250	58.710	13.526	24.523	1.00	27.61	6
	ATOM	4040	C	THR	B	250	60.191	13.683	24.413	1.00	26.93	6
	ATOM	4041	O	THR	B	250	60.785	14.328	23.570	1.00	28.19	8
	ATOM	4042	CB	THR	B	250	58.162	14.831	25.186	1.00	30.35	6
	ATOM	4043	OG1	THR	B	250	58.797	14.978	26.457	1.00	31.06	8
45	ATOM	4044	CG2	THR	B	250	56.677	14.760	25.380	1.00	32.40	6
	ATOM	4045	N	LEU	B	251	60.891	12.958	25.324	1.00	27.41	7
	ATOM	4046	CA	LEU	B	251	62.336	12.857	25.461	1.00	30.17	6
	ATOM	4047	C	LEU	B	251	62.928	14.204	25.968	1.00	31.32	6
	ATOM	4048	O	LEU	B	251	64.110	14.434	25.775	1.00	33.84	8
50	ATOM	4049	CB	LEU	B	251	63.096	12.483	24.205	1.00	30.53	6
	ATOM	4050	CG	LEU	B	251	62.568	11.151	23.560	1.00	30.23	6
	ATOM	4051	CD1	LEU	B	251	63.382	10.891	22.307	1.00	31.95	6
	ATOM	4052	CD2	LEU	B	251	62.575	10.004	24.541	1.00	30.44	6
	ATOM	4053	N	LEU	B	252	62.054	15.017	26.483	1.00	33.09	7
55	ATOM	4054	CA	LEU	B	252	62.441	16.323	27.015	1.00	34.68	6
	ATOM	4055	C	LEU	B	252	62.530	16.162	28.519	1.00	35.10	6
	ATOM	4056	O	LEU	B	252	62.436	15.037	29.003	1.00	30.04	8
	ATOM	4057	CB	LEU	B	252	61.439	17.401	26.633	1.00	35.48	6
	ATOM	4058	CG	LEU	B	252	61.476	17.664	25.106	1.00	38.16	6
60	ATOM	4059	CD1	LEU	B	252	60.219	18.416	24.715	1.00	38.56	6
	ATOM	4060	CD2	LEU	B	252	62.782	18.361	24.789	1.00	38.57	6
	ATOM	4061	N	GLU	B	253	62.625	17.316	29.217	1.00	36.82	7
	ATOM	4062	CA	GLU	B	253	62.731	17.220	30.668	1.00	39.59	6
	ATOM	4063	C	GLU	B	253	61.417	16.777	31.259	1.00	39.50	6
65	ATOM	4064	O	GLU	B	253	60.403	17.042	30.591	1.00	40.91	8
	ATOM	4065	CB	GLU	B	253	63.103	18.586	31.274	1.00	42.93	6
	ATOM	4066	CG	GLU	B	253	64.342	19.202	30.643	1.00	48.27	6
	ATOM	4067	CD	GLU	B	253	65.560	18.356	30.999	1.00	51.88	6
	ATOM	4068	OE1	GLU	B	253	65.758	18.143	32.226	1.00	54.42	8
70	ATOM	4069	OE2	GLU	B	253	66.259	17.915	30.063	1.00	53.71	8
	ATOM	4070	N	VAL	B	254	61.405	16.130	32.403	1.00	39.00	7
	ATOM	4071	CA	VAL	B	254	60.167	15.751	33.062	1.00	40.35	6
	ATOM	4072	C	VAL	B	254	59.384	16.991	33.488	1.00	43.05	6
	ATOM	4073	O	VAL	B	254	59.955	17.997	33.903	1.00	42.79	8
	ATOM	4074	CB	VAL	B	254	60.425	14.856	34.285	1.00	39.32	6

-92-

	ATOM	4075	CG1	VAL	B	254	59.162	14.614	35.088	1.00	37.70	6
	ATOM	4076	CG2	VAL	B	254	61.054	13.553	33.783	1.00	38.29	6
	ATOM	4077	N	SER	B	255	58.070	16.937	33.293	1.00	46.50	7
5	ATOM	4078	CA	SER	B	255	57.178	18.041	33.641	1.00	47.57	6
	ATOM	4079	C	SER	B	255	56.027	17.520	34.498	1.00	48.72	6
	ATOM	4080	O	SER	B	255	56.063	16.436	35.062	1.00	49.33	8
	ATOM	4081	CB	SER	B	255	56.663	18.739	32.379	1.00	47.97	6
	ATOM	4082	OG	SER	B	255	55.566	18.022	31.814	1.00	50.04	8
10	ATOM	4083	N	GLU	B	256	54.990	18.358	34.593	1.00	48.58	7
	ATOM	4084	CA	GLU	B	256	53.787	18.010	35.346	1.00	49.19	6
	ATOM	4085	C	GLU	B	256	52.838	17.201	34.488	1.00	49.15	6
	ATOM	4086	O	GLU	B	256	51.953	16.493	34.969	1.00	50.39	8
	ATOM	4087	CB	GLU	B	256	53.154	19.321	35.844	1.00	49.68	6
15	ATOM	4088	N	THR	B	257	53.078	17.241	33.177	1.00	48.71	7
	ATOM	4089	CA	THR	B	257	52.306	16.471	32.211	1.00	49.54	6
	ATOM	4090	C	THR	B	257	52.962	15.121	31.914	1.00	48.26	6
	ATOM	4091	O	THR	B	257	52.333	14.259	31.285	1.00	48.37	8
	ATOM	4092	CB	THR	B	257	52.146	17.265	30.913	1.00	50.65	6
20	ATOM	4093	OG1	THR	B	257	53.430	17.717	30.454	1.00	52.73	8
	ATOM	4094	CG2	THR	B	257	51.277	18.496	31.154	1.00	52.44	6
	ATOM	4095	N	SER	B	258	54.201	14.933	32.368	1.00	44.00	7
	ATOM	4096	CA	SER	B	258	54.923	13.690	32.124	1.00	43.02	6
	ATOM	4097	C	SER	B	258	54.197	12.470	32.665	1.00	41.05	6
25	ATOM	4098	O	SER	B	258	53.785	12.435	33.808	1.00	40.25	8
	ATOM	4099	CB	SER	B	258	56.315	13.710	32.765	1.00	39.95	6
	ATOM	4100	OG	SER	B	258	57.171	14.561	32.020	1.00	37.63	8
	ATOM	4101	N	LYS	B	259	54.041	11.453	31.819	1.00	40.55	7
	ATOM	4102	CA	LYS	B	259	53.347	10.253	32.275	1.00	40.93	6
30	ATOM	4103	C	LYS	B	259	54.339	9.094	32.390	1.00	38.96	6
	ATOM	4104	O	LYS	B	259	54.036	8.130	33.071	1.00	39.56	8
	ATOM	4105	CB	LYS	B	259	52.193	9.870	31.340	1.00	44.20	6
	ATOM	4106	CG	LYS	B	259	51.223	11.038	31.184	1.00	47.43	6
	ATOM	4107	CD	LYS	B	259	49.868	10.656	30.608	1.00	50.95	6
35	ATOM	4108	CE	LYS	B	259	48.814	11.646	31.143	1.00	52.15	6
	ATOM	4109	NZ	LYS	B	259	47.678	11.728	30.177	1.00	54.34	7
	ATOM	4110	N	ARG	B	260	55.446	9.187	31.695	1.00	38.03	7
	ATOM	4111	CA	ARG	B	260	56.469	8.146	31.706	1.00	36.81	6
	ATOM	4112	C	ARG	B	260	57.852	8.765	31.794	1.00	33.36	6
40	ATOM	4113	O	ARG	B	260	58.150	9.717	31.075	1.00	30.91	8
	ATOM	4114	CB	ARG	B	260	56.438	7.267	30.445	1.00	38.22	6
	ATOM	4115	CG	ARG	B	260	55.182	6.504	30.103	1.00	42.83	6
	ATOM	4116	CD	ARG	B	260	55.389	5.584	28.896	1.00	43.79	6
	ATOM	4117	NE	ARG	B	260	54.174	4.856	28.536	1.00	46.34	7
45	ATOM	4118	N	ALA	B	261	58.808	8.142	32.519	1.00	31.91	7
	ATOM	4119	CA	ALA	B	261	60.182	8.623	32.486	1.00	28.39	6
	ATOM	4120	C	ALA	B	261	61.176	7.524	32.106	1.00	25.89	6
	ATOM	4121	O	ALA	B	261	60.882	6.354	32.381	1.00	29.01	8
	ATOM	4122	CB	ALA	B	261	60.695	9.169	33.836	1.00	29.25	6
50	ATOM	4123	N	VAL	B	262	62.238	7.874	31.454	1.00	27.17	7
	ATOM	4124	CA	VAL	B	262	63.325	6.947	31.122	1.00	29.12	6
	ATOM	4125	C	VAL	B	262	64.544	7.432	31.944	1.00	28.50	6
	ATOM	4126	O	VAL	B	262	64.860	8.605	31.932	1.00	27.83	8
	ATOM	4127	CB	VAL	B	262	63.659	6.838	29.647	1.00	30.51	6
55	ATOM	4128	CG1	VAL	B	262	63.902	8.231	29.043	1.00	30.91	6
	ATOM	4129	CG2	VAL	B	262	64.881	5.958	29.356	1.00	30.63	6
	ATOM	4130	N	ILE	B	263	65.221	6.505	32.611	1.00	29.18	7
	ATOM	4131	CA	ILE	B	263	66.406	6.792	33.454	1.00	27.39	6
	ATOM	4132	C	ILE	B	263	67.590	6.119	32.790	1.00	25.94	6
60	ATOM	4133	O	ILE	B	263	67.437	4.906	32.507	1.00	25.04	8
	ATOM	4134	CB	ILE	B	263	66.243	6.278	34.881	1.00	29.45	6
	ATOM	4135	CG1	ILE	B	263	64.898	6.687	35.497	1.00	29.18	6
	ATOM	4136	CG2	ILE	B	263	67.369	6.819	35.758	1.00	29.13	6
	ATOM	4137	CD1	ILE	B	263	64.395	5.672	36.508	1.00	32.09	6
65	ATOM	4138	N	LEU	B	264	68.626	6.784	32.377	1.00	25.66	7
	ATOM	4139	CA	LEU	B	264	69.795	6.289	31.701	1.00	27.04	6
	ATOM	4140	C	LEU	B	264	70.978	6.430	32.666	1.00	29.07	6
	ATOM	4141	O	LEU	B	264	71.152	7.574	33.143	1.00	29.50	8
	ATOM	4142	CB	LEU	B	264	70.153	7.070	30.438	1.00	29.75	6
70	ATOM	4143	CG	LEU	B	264	68.950	7.229	29.452	1.00	32.20	6
	ATOM	4144	CD1	LEU	B	264	69.399	8.095	28.298	1.00	33.01	6
	ATOM	4145	CD2	LEU	B	264	68.453	5.842	29.091	1.00	31.89	6
	ATOM	4146	N	VAL	B	265	71.753	5.394	32.886	1.00	29.03	7
	ATOM	4147	CA	VAL	B	265	72.864	5.494	33.821	1.00	32.13	6
	ATOM	4148	C	VAL	B	265	74.099	4.822	33.213	1.00	34.01	6

	ATOM	4149	O	VAL	B	265	74.044	3.750	32.557	1.00	34.46	8
	ATOM	4150	CB	VAL	B	265	72.642	4.856	35.202	1.00	32.74	6
	ATOM	4151	CG1	VAL	B	265	71.525	5.474	36.025	1.00	33.45	6
5	ATOM	4152	CG2	VAL	B	265	72.331	3.361	35.046	1.00	33.30	6
	ATOM	4153	N	ALA	B	266	75.219	5.485	33.397	1.00	33.41	7
	ATOM	4154	CA	ALA	B	266	76.501	4.926	33.000	1.00	32.14	6
	ATOM	4155	C	ALA	B	266	77.411	5.092	34.221	1.00	32.17	6
	ATOM	4156	O	ALA	B	266	77.390	6.213	34.746	1.00	32.13	8
10	ATOM	4157	CB	ALA	B	266	77.139	5.570	31.794	1.00	32.99	6
	ATOM	4158	N	ALA	B	267	78.175	4.058	34.569	1.00	31.42	7
	ATOM	4159	CA	ALA	B	267	79.107	4.338	35.679	1.00	32.75	6
	ATOM	4160	C	ALA	B	267	80.356	3.503	35.491	1.00	35.34	6
	ATOM	4161	O	ALA	B	267	80.213	2.423	34.884	1.00	36.90	8
15	ATOM	4162	CB	ALA	B	267	78.446	4.006	36.993	1.00	31.22	6
	ATOM	4163	N	TRP	B	268	81.511	3.868	36.036	1.00	36.69	7
	ATOM	4164	CA	TRP	B	268	82.665	2.974	35.881	1.00	38.65	6
	ATOM	4165	C	TRP	B	268	82.910	2.113	37.105	1.00	40.28	6
	ATOM	4166	O	TRP	B	268	82.777	2.579	38.235	1.00	38.57	8
20	ATOM	4167	CB	TRP	B	268	83.927	3.805	35.609	1.00	40.65	6
	ATOM	4168	CG	TRP	B	268	83.860	4.563	34.319	1.00	43.80	6
	ATOM	4169	CD1	TRP	B	268	83.114	5.662	34.040	1.00	44.47	6
	ATOM	4170	CD2	TRP	B	268	84.577	4.256	33.115	1.00	45.14	6
	ATOM	4171	NE1	TRP	B	268	83.311	6.063	32.729	1.00	45.41	7
25	ATOM	4172	CE2	TRP	B	268	84.199	5.211	32.144	1.00	45.95	6
	ATOM	4173	CE3	TRP	B	268	85.470	3.244	32.757	1.00	45.65	6
	ATOM	4174	CZ2	TRP	B	268	84.703	5.199	30.836	1.00	46.17	6
	ATOM	4175	CZ3	TRP	B	268	85.984	3.242	31.463	1.00	46.00	6
	ATOM	4176	CH2	TRP	B	268	85.596	4.206	30.522	1.00	45.63	6
30	ATOM	4177	N	LEU	B	269	83.300	0.869	36.821	1.00	39.18	7
	ATOM	4178	CA	LEU	B	269	83.691	-0.026	37.916	1.00	43.86	6
	ATOM	4179	C	LEU	B	269	85.093	-0.471	37.522	1.00	46.33	6
	ATOM	4180	O	LEU	B	269	85.247	-0.946	36.400	1.00	47.07	8
	ATOM	4181	CB	LEU	B	269	82.635	-1.086	38.058	1.00	43.77	6
35	ATOM	4182	CG	LEU	B	269	82.651	-2.072	39.212	1.00	44.62	6
	ATOM	4183	CD1	LEU	B	269	82.571	-1.312	40.537	1.00	44.46	6
	ATOM	4184	CD2	LEU	B	269	81.518	-3.080	39.046	1.00	42.39	6
	ATOM	4185	N	GLY	B	270	86.102	-0.049	38.293	1.00	48.41	7
	ATOM	4186	CA	GLY	B	270	87.475	-0.340	37.862	1.00	51.49	6
40	ATOM	4187	C	GLY	B	270	87.681	0.391	36.532	1.00	54.10	6
	ATOM	4188	O	GLY	B	270	87.397	1.588	36.464	1.00	54.18	8
	ATOM	4189	N	ASP	B	271	88.108	-0.331	35.503	1.00	56.24	7
	ATOM	4190	CA	ASP	B	271	88.288	0.320	34.199	1.00	56.89	6
	ATOM	4191	C	ASP	B	271	87.142	-0.096	33.280	1.00	54.99	6
45	ATOM	4192	O	ASP	B	271	87.162	0.231	32.097	1.00	55.57	8
	ATOM	4193	CB	ASP	B	271	89.670	0.026	33.618	1.00	60.69	6
	ATOM	4194	CG	ASP	B	271	90.400	-1.175	34.164	1.00	64.16	6
	ATOM	4195	OD1	ASP	B	271	89.789	-2.194	34.571	1.00	65.71	8
	ATOM	4196	OD2	ASP	B	271	91.657	-1.179	34.206	1.00	66.40	8
50	ATOM	4197	N	ALA	B	272	86.129	-0.780	33.807	1.00	52.97	7
	ATOM	4198	CA	ALA	B	272	84.966	-1.186	33.031	1.00	50.67	6
	ATOM	4199	C	ALA	B	272	83.843	-0.149	33.103	1.00	50.64	6
	ATOM	4200	O	ALA	B	272	83.482	0.315	34.203	1.00	49.32	8
	ATOM	4201	CB	ALA	B	272	84.389	-2.501	33.520	1.00	50.42	6
55	ATOM	4202	N	ARG	B	273	83.255	0.166	31.958	1.00	47.60	7
	ATOM	4203	CA	ARG	B	273	82.163	1.131	31.939	1.00	46.77	6
	ATOM	4204	C	ARG	B	273	80.841	0.398	31.804	1.00	45.84	6
	ATOM	4205	O	ARG	B	273	80.636	-0.256	30.770	1.00	46.17	8
	ATOM	4206	CB	ARG	B	273	82.312	2.144	30.804	1.00	48.87	6
60	ATOM	4207	CG	ARG	B	273	81.234	3.214	30.839	1.00	49.86	6
	ATOM	4208	CD	ARG	B	273	81.436	4.283	29.773	1.00	52.81	6
	ATOM	4209	NE	ARG	B	273	80.277	5.174	29.733	1.00	54.38	7
	ATOM	4210	CZ	ARG	B	273	79.665	5.669	28.671	1.00	55.34	6
	ATOM	4211	NH1	ARG	B	273	80.083	5.410	27.433	1.00	56.45	7
65	ATOM	4212	NH2	ARG	B	273	78.606	6.455	28.819	1.00	54.66	7
	ATOM	4213	N	LEU	B	274	79.992	0.448	32.821	1.00	41.38	7
	ATOM	4214	CA	LEU	B	274	78.715	-0.229	32.792	1.00	37.98	6
	ATOM	4215	C	LEU	B	274	77.584	0.737	32.506	1.00	37.26	6
	ATOM	4216	O	LEU	B	274	77.586	1.908	32.909	1.00	36.11	8
70	ATOM	4217	CB	LEU	B	274	78.395	-0.939	34.118	1.00	38.68	6
	ATOM	4218	CG	LEU	B	274	79.554	-1.797	34.654	1.00	41.26	6
	ATOM	4219	CD1	LEU	B	274	79.161	-2.469	35.960	1.00	41.73	6
	ATOM	4220	CD2	LEU	B	274	79.999	-2.827	33.625	1.00	42.85	6
	ATOM	4221	N	ILE	B	275	76.603	0.270	31.724	1.00	35.74	7
	ATOM	4222	CA	ILE	B	275	75.493	1.141	31.372	1.00	33.53	6

-94-

5	ATOM	4223	C	ILE	B	275	74.202	-0.402	-31.685	1.00	32.45	6
	ATOM	4224	O	ILE	B	275	74.121	-0.836	31.733	1.00	31.50	8
	ATOM	4225	CB	ILE	B	275	75.466	1.658	29.914	1.00	36.92	6
	ATOM	4226	CG1	ILE	B	275	75.105	0.527	28.946	1.00	37.93	6
	ATOM	4227	CG2	ILE	B	275	76.794	2.331	29.537	1.00	36.91	6
	ATOM	4228	CD1	ILE	B	275	74.962	1.004	27.506	1.00	38.53	6
	ATOM	4229	N	ASP	B	276	73.124	1.174	31.933	1.00	28.46	7
	ATOM	4230	CA	ASP	B	276	71.866	0.517	32.262	1.00	30.30	6
10	ATOM	4231	C	ASP	B	276	70.716	1.517	32.068	1.00	29.63	6
	ATOM	4232	O	ASP	B	276	71.081	2.666	31.835	1.00	27.88	8
	ATOM	4233	CB	ASP	B	276	71.937	-0.066	33.671	1.00	32.97	6
	ATOM	4234	CG	ASP	B	276	70.851	-1.058	33.987	1.00	34.63	6
	ATOM	4235	OD1	ASP	B	276	69.857	-1.272	33.231	1.00	37.08	8
15	ATOM	4236	OD2	ASP	B	276	70.931	-1.716	35.054	1.00	35.37	8
	ATOM	4237	N	ASN	B	277	69.478	1.072	32.012	1.00	30.76	7
	ATOM	4238	CA	ASN	B	277	68.339	1.963	31.738	1.00	31.92	6
	ATOM	4239	C	ASN	B	277	67.121	1.388	32.426	1.00	29.27	6
	ATOM	4240	O	ASN	B	277	67.035	0.187	32.641	1.00	30.64	8
20	ATOM	4241	CB	ASN	B	277	68.041	2.214	30.258	1.00	37.99	6
	ATOM	4242	CG	ASN	B	277	66.700	1.999	29.601	1.00	41.20	6
	ATOM	4243	OD1	ASN	B	277	65.702	1.397	30.046	1.00	41.98	8
	ATOM	4244	ND2	ASN	B	277	66.503	2.495	28.345	1.00	41.86	7
	ATOM	4245	N	LYS	B	278	66.149	2.219	32.760	1.00	28.29	7
25	ATOM	4246	CA	LYS	B	278	64.891	1.736	33.328	1.00	30.58	6
	ATOM	4247	C	LYS	B	278	63.822	2.756	32.929	1.00	33.32	6
	ATOM	4248	O	LYS	B	278	64.130	3.940	32.793	1.00	32.01	8
	ATOM	4249	CB	LYS	B	278	64.919	1.486	34.834	1.00	31.32	6
	ATOM	4250	CG	LYS	B	278	63.617	0.953	35.422	1.00	35.08	6
30	ATOM	4251	CD	LYS	B	278	63.793	0.340	36.790	1.00	38.13	6
	ATOM	4252	CE	LYS	B	278	63.031	-0.950	37.108	1.00	39.29	6
	ATOM	4253	NZ	LYS	B	278	63.193	-1.103	38.612	1.00	44.44	7
	ATOM	4254	N	MET	B	279	62.625	2.256	32.594	1.00	33.66	7
	ATOM	4255	CA	MET	B	279	61.488	3.102	32.303	1.00	36.39	6
35	ATOM	4256	C	MET	B	279	60.543	3.014	33.483	1.00	35.26	6
	ATOM	4257	O	MET	B	279	60.470	1.929	34.090	1.00	38.21	8
	ATOM	4258	CB	MET	B	279	60.797	2.708	30.965	1.00	38.06	6
	ATOM	4259	CG	MET	B	279	61.358	3.604	29.846	1.00	42.01	6
	ATOM	4260	SD	MET	B	279	61.219	2.888	28.222	1.00	48.77	16
40	ATOM	4261	CE	MET	B	279	62.632	3.595	27.392	1.00	46.06	6
	ATOM	4262	N	VAL	B	280	59.853	4.082	33.859	1.00	34.69	7
	ATOM	4263	CA	VAL	B	280	58.937	4.046	34.991	1.00	37.86	6
	ATOM	4264	C	VAL	B	280	57.655	4.778	34.624	1.00	39.91	6
	ATOM	4265	O	VAL	B	280	57.722	5.842	33.971	1.00	39.57	8
45	ATOM	4266	CB	VAL	B	280	59.605	4.627	36.262	1.00	40.03	6
	ATOM	4267	CG1	VAL	B	280	60.582	5.734	35.894	1.00	40.43	6
	ATOM	4268	CG2	VAL	B	280	58.595	5.132	37.286	1.00	41.28	6
	ATOM	4269	N	GLU	B	281	56.521	4.221	35.046	1.00	42.47	7
	ATOM	4270	CA	GLU	B	281	55.243	4.911	34.809	1.00	45.74	6
50	ATOM	4271	C	GLU	B	281	54.973	5.919	35.910	1.00	47.07	6
	ATOM	4272	O	GLU	B	281	55.370	5.595	37.039	1.00	46.25	8
	ATOM	4273	CB	GLU	B	281	54.152	3.848	34.719	1.00	47.41	6
	ATOM	4274	CG	GLU	B	281	54.308	2.918	33.516	1.00	48.19	6
	ATOM	4275	CD	GLU	B	281	53.705	3.562	32.275	1.00	50.10	6
55	ATOM	4276	OE1	GLU	B	281	52.718	4.312	32.460	1.00	51.21	8
	ATOM	4277	OE2	GLU	B	281	54.203	3.330	31.153	1.00	50.72	8
	ATOM	4278	N	LEU	B	282	54.358	7.077	35.662	1.00	49.43	7
	ATOM	4279	CA	LEU	B	282	54.144	8.043	36.731	1.00	52.69	6
	ATOM	4280	C	LEU	B	282	52.714	8.211	37.222	1.00	56.10	6
60	ATOM	4281	O	LEU	B	282	51.741	8.259	36.479	1.00	57.86	8
	ATOM	4282	CB	LEU	B	282	54.654	9.413	36.232	1.00	51.33	6
	ATOM	4283	CG	LEU	B	282	56.153	9.442	35.898	1.00	51.16	6
	ATOM	4284	CD1	LEU	B	282	56.568	10.774	35.313	1.00	49.90	6
	ATOM	4285	CD2	LEU	B	282	56.959	9.109	37.146	1.00	50.87	6
65	ATOM	4286	N	ALA	B	283	52.591	8.404	38.527	1.00	58.60	7
	ATOM	4287	CA	ALA	B	283	51.340	8.572	39.260	1.00	61.51	6
	ATOM	4288	C	ALA	B	283	50.222	7.659	38.748	1.00	62.69	6
	ATOM	4289	O	ALA	B	283	49.365	7.240	39.565	1.00	64.21	8
	ATOM	4290	CB	ALA	B	283	50.878	10.031	39.215	1.00	61.28	

70

Water

Atom	X	Y	Z	Occ.	B
------	---	---	---	------	---

type

	ATOM	4303	O	WAT	W	1	33.957	17.885	-21.689	1.00	20.48
5	ATOM	4304	O	WAT	W	2	37.847	13.185	4.982	1.00	21.45
	ATOM	4305	O	WAT	W	3	63.980	-1.350	11.191	1.00	28.46
	ATOM	4306	O	WAT	W	4	56.095	-1.331	-2.328	1.00	33.26
	ATOM	4307	O	WAT	W	5	33.170	18.137	-24.293	1.00	23.96
	ATOM	4308	O	WAT	W	6	37.215	10.622	-2.497	1.00	25.23
10	ATOM	4309	O	WAT	W	7	34.408	20.030	-20.099	1.00	22.90
	ATOM	4310	O	WAT	W	8	44.843	0.417	12.211	1.00	25.44
	ATOM	4311	O	WAT	W	9	32.057	20.794	-18.723	1.00	21.33
	ATOM	4312	O	WAT	W	10	39.891	15.086	5.128	1.00	21.17
	ATOM	4313	O	WAT	W	11	60.554	9.975	11.882	1.00	23.86
15	ATOM	4314	O	WAT	W	12	47.956	16.767	16.754	1.00	25.70
	ATOM	4315	O	WAT	W	13	26.013	19.028	0.123	1.00	29.25
	ATOM	4316	O	WAT	W	14	41.289	15.802	-0.016	1.00	29.45
	ATOM	4317	O	WAT	W	15	26.238	26.828	-12.429	1.00	26.43
	ATOM	4318	O	WAT	W	16	42.677	-8.069	14.438	1.00	49.57
20	ATOM	4319	O	WAT	W	17	44.205	-22.405	7.937	1.00	26.54
	ATOM	4320	O	WAT	W	18	41.204	15.438	2.596	1.00	28.73
	ATOM	4321	O	WAT	W	19	50.665	6.851	-9.161	1.00	28.82
	ATOM	4322	O	WAT	W	20	45.856	11.020	16.763	1.00	28.19
	ATOM	4323	O	WAT	W	21	56.240	9.146	22.228	1.00	29.25
25	ATOM	4324	O	WAT	W	22	34.167	22.025	-17.131	1.00	24.52
	ATOM	4325	O	WAT	W	23	46.937	-3.706	12.756	1.00	34.74
	ATOM	4326	O	WAT	W	24	42.413	2.422	14.402	1.00	33.61
	ATOM	4327	O	WAT	W	25	41.229	-21.204	14.206	1.00	24.13
	ATOM	4328	O	WAT	W	26	41.221	12.093	-6.937	1.00	25.26
30	ATOM	4329	O	WAT	W	27	24.372	15.958	-5.041	1.00	27.65
	ATOM	4330	O	WAT	W	28	35.615	-12.052	11.939	1.00	30.34
	ATOM	4331	O	WAT	W	29	37.895	12.192	-4.849	1.00	26.69
	ATOM	4332	O	WAT	W	30	52.106	20.252	-2.182	1.00	28.30
	ATOM	4333	O	WAT	W	31	68.369	9.094	44.468	1.00	25.44
35	ATOM	4334	O	WAT	W	32	56.344	0.572	-4.129	1.00	43.47
	ATOM	4335	O	WAT	W	33	23.101	20.797	-4.005	1.00	36.59
	ATOM	4336	O	WAT	W	34	49.261	-5.331	2.868	1.00	26.99
	ATOM	4337	O	WAT	W	35	47.984	-9.414	25.007	1.00	26.83
	ATOM	4338	O	WAT	W	36	42.604	-1.487	5.352	1.00	30.62
40	ATOM	4339	O	WAT	W	37	62.274	-5.597	10.141	1.00	27.42
	ATOM	4340	O	WAT	W	38	26.216	16.962	-12.131	1.00	28.51
	ATOM	4341	O	WAT	W	39	30.958	20.957	-10.945	1.00	28.67
	ATOM	4342	O	WAT	W	40	34.816	15.313	17.023	1.00	30.79
	ATOM	4343	O	WAT	W	41	49.918	15.022	17.578	1.00	28.50
45	ATOM	4344	O	WAT	W	42	51.910	5.889	8.625	1.00	38.44
	ATOM	4345	O	WAT	W	43	62.846	-1.187	14.226	1.00	46.50
	ATOM	4346	O	WAT	W	44	25.403	26.593	-16.292	1.00	39.06
	ATOM	4347	O	WAT	W	45	30.520	20.301	5.385	1.00	32.49
	ATOM	4348	O	WAT	W	46	45.010	-17.167	2.635	1.00	34.22
50	ATOM	4349	O	WAT	W	47	47.032	-2.770	5.031	1.00	22.23
	ATOM	4350	O	WAT	W	48	48.414	1.477	-5.713	1.00	29.51
	ATOM	4351	O	WAT	W	49	31.672	7.463	-13.621	1.00	36.04
	ATOM	4352	O	WAT	W	50	62.969	0.366	20.839	1.00	25.12
	ATOM	4353	O	WAT	W	51	52.181	16.341	18.209	1.00	33.67
55	ATOM	4354	O	WAT	W	52	34.216	17.207	10.342	1.00	25.68
	ATOM	4355	O	WAT	W	53	52.739	13.892	-0.142	1.00	24.81
	ATOM	4356	O	WAT	W	54	48.513	-7.403	4.595	1.00	33.10
	ATOM	4357	O	WAT	W	55	50.165	3.786	7.424	1.00	31.96
	ATOM	4358	O	WAT	W	56	61.601	-10.884	-3.900	1.00	38.55
60	ATOM	4359	O	WAT	W	57	40.862	-13.477	5.834	1.00	26.78
	ATOM	4360	O	WAT	W	58	73.540	-3.703	38.069	1.00	28.56
	ATOM	4361	O	WAT	W	59	53.267	18.858	-0.006	1.00	28.15
	ATOM	4362	O	WAT	W	60	47.896	-10.104	11.452	1.00	29.42
	ATOM	4363	O	WAT	W	61	32.210	13.233	-12.282	1.00	31.94
65	ATOM	4364	O	WAT	W	62	48.007	11.908	18.269	1.00	37.69
	ATOM	4365	O	WAT	W	63	29.173	9.259	-17.716	1.00	30.38
	ATOM	4366	O	WAT	W	64	35.297	19.389	9.031	1.00	29.80
	ATOM	4367	O	WAT	W	65	40.504	2.299	-10.545	1.00	32.49
	ATOM	4368	O	WAT	W	66	41.958	-10.772	13.351	1.00	42.64
70	ATOM	4369	O	WAT	W	67	36.143	16.525	-1.066	1.00	34.59
	ATOM	4370	O	WAT	W	68	62.385	-11.067	-1.312	1.00	33.16
	ATOM	4371	O	WAT	W	69	65.110	11.392	10.350	1.00	28.97
	ATOM	4372	O	WAT	W	70	63.427	-3.415	19.364	1.00	27.45
	ATOM	4373	O	WAT	W	71	68.617	14.525	33.511	1.00	37.55
	ATOM	4374	O	WAT	W	72	61.639	-4.893	17.918	1.00	24.98

-96-

	ATOM	4375	O	WAT	W	73	66.736	4.204	19.794	1.00	30.21
	ATOM	4376	O	WAT	W	74	55.982	12.796	22.001	1.00	36.21
	ATOM	4377	O	WAT	W	75	64.346	6.123	-5.386	1.00	40.37
5	ATOM	4378	O	WAT	W	76	65.025	-2.313	32.956	1.00	37.41
	ATOM	4379	O	WAT	W	77	44.448	-0.359	-6.294	1.00	29.00
	ATOM	4380	O	WAT	W	78	48.675	-0.966	-4.566	1.00	35.26
	ATOM	4381	O	WAT	W	79	31.748	14.620	-27.469	1.00	30.01
	ATOM	4382	O	WAT	W	80	22.272	14.300	-4.370	1.00	33.41
10	ATOM	4383	O	WAT	W	81	61.185	6.162	25.319	1.00	33.42
	ATOM	4384	O	WAT	W	82	25.793	11.693	-9.261	1.00	32.09
	ATOM	4385	O	WAT	W	83	44.087	16.403	-7.636	1.00	30.17
	ATOM	4386	O	WAT	W	84	42.576	-4.126	6.016	1.00	55.25
	ATOM	4387	O	WAT	W	85	68.891	7.733	20.798	1.00	37.85
15	ATOM	4388	O	WAT	W	86	70.712	-5.611	41.295	1.00	34.04
	ATOM	4389	O	WAT	W	87	43.384	-22.647	14.391	1.00	41.78
	ATOM	4390	O	WAT	W	88	70.983	-8.966	9.646	1.00	33.63
	ATOM	4391	O	WAT	W	89	75.957	-17.895	11.852	1.00	47.71
	ATOM	4392	O	WAT	W	90	63.730	-0.759	18.432	1.00	34.78
20	ATOM	4393	O	WAT	W	91	31.689	15.534	-14.467	1.00	32.23
	ATOM	4394	O	WAT	W	92	44.527	-11.830	12.755	1.00	34.17
	ATOM	4395	O	WAT	W	93	20.677	30.620	-24.626	1.00	31.71
	ATOM	4396	O	WAT	W	94	44.639	17.338	-10.200	1.00	34.48
	ATOM	4397	O	WAT	W	95	75.731	12.312	36.456	1.00	43.57
25	ATOM	4398	O	WAT	W	96	44.412	10.904	19.269	1.00	42.19
	ATOM	4399	O	WAT	W	97	22.294	30.665	-27.831	1.00	34.67
	ATOM	4400	O	WAT	W	98	61.020	1.839	-4.047	1.00	32.70
	ATOM	4401	O	WAT	W	99	63.564	-3.241	9.033	1.00	26.37
	ATOM	4402	O	WAT	W	100	58.754	3.167	-4.838	1.00	32.36
30	ATOM	4403	O	WAT	W	101	65.772	-9.474	4.700	1.00	28.90
	ATOM	4404	O	WAT	W	102	68.154	15.020	30.966	1.00	48.55
	ATOM	4405	O	WAT	W	103	69.423	3.142	26.541	1.00	37.38
	ATOM	4406	O	WAT	W	104	46.011	16.393	-32.096	1.00	35.12
	ATOM	4407	O	WAT	W	105	29.379	18.412	-31.086	1.00	39.01
35	ATOM	4408	O	WAT	W	106	45.917	-11.276	10.149	1.00	27.62
	ATOM	4409	O	WAT	W	107	24.739	28.644	-17.280	1.00	32.77
	ATOM	4410	O	WAT	W	108	79.205	12.257	45.859	1.00	41.16
	ATOM	4411	O	WAT	W	109	73.058	-3.265	35.431	1.00	33.63
	ATOM	4412	O	WAT	W	110	46.854	-9.240	3.826	1.00	36.79
40	ATOM	4413	O	WAT	W	111	25.850	9.001	-9.625	1.00	34.69
	ATOM	4414	O	WAT	W	112	62.047	8.655	0.423	1.00	33.56
	ATOM	4415	O	WAT	W	113	37.663	10.928	-18.842	1.00	34.05
	ATOM	4416	O	WAT	W	114	34.619	21.383	-14.295	1.00	30.74
	ATOM	4417	O	WAT	W	115	58.523	21.835	-8.875	1.00	37.34
45	ATOM	4418	O	WAT	W	116	28.178	28.182	-10.656	1.00	43.64
	ATOM	4419	O	WAT	W	117	66.395	-3.417	24.653	1.00	32.24
	ATOM	4420	O	WAT	W	118	51.651	21.138	16.503	1.00	35.04
	ATOM	4421	O	WAT	W	119	46.184	-9.790	13.725	1.00	38.61
	ATOM	4422	O	WAT	W	120	77.317	-2.960	44.894	1.00	29.27
50	ATOM	4423	O	WAT	W	121	53.189	17.937	10.605	1.00	29.73
	ATOM	4424	O	WAT	W	122	36.010	12.829	-10.679	1.00	33.47
	ATOM	4425	O	WAT	W	123	34.086	3.401	-11.327	1.00	50.83
	ATOM	4426	O	WAT	W	124	67.551	-6.941	-3.458	1.00	40.00
	ATOM	4427	O	WAT	W	125	22.839	14.210	-21.134	1.00	33.56
55	ATOM	4428	O	WAT	W	126	46.144	1.450	-7.279	1.00	34.78
	ATOM	4429	O	WAT	W	127	44.101	21.525	16.698	1.00	39.31
	ATOM	4430	O	WAT	W	128	53.306	5.434	-16.838	1.00	54.57
	ATOM	4431	O	WAT	W	129	50.250	1.205	22.740	1.00	28.98
	ATOM	4432	O	WAT	W	130	26.485	19.155	-29.949	1.00	29.98
60	ATOM	4433	O	WAT	W	131	24.707	18.542	-27.822	1.00	37.35
	ATOM	4434	O	WAT	W	132	67.710	5.567	21.896	1.00	29.04
	ATOM	4435	O	WAT	W	133	45.674	-4.052	19.840	1.00	36.16
	ATOM	4436	O	WAT	W	134	24.220	25.124	-21.068	1.00	34.59
	ATOM	4437	O	WAT	W	135	61.598	17.680	13.540	1.00	42.71
65	ATOM	4438	O	WAT	W	136	49.468	-7.110	25.310	1.00	38.94
	ATOM	4439	O	WAT	W	137	66.911	11.234	12.429	1.00	37.05
	ATOM	4440	O	WAT	W	138	57.148	2.737	30.896	1.00	48.38
	ATOM	4441	O	WAT	W	139	34.489	9.771	-18.467	1.00	30.91
	ATOM	4442	O	WAT	W	140	32.760	21.132	4.304	1.00	29.66
70	ATOM	4443	O	WAT	W	141	49.857	-2.000	-1.297	1.00	39.89
	ATOM	4444	O	WAT	W	142	54.890	-1.411	27.207	1.00	47.87
	ATOM	4445	O	WAT	W	143	64.172	15.675	32.993	1.00	36.07
	ATOM	4446	O	WAT	W	144	55.868	-7.470	-4.555	1.00	42.27
	ATOM	4447	O	WAT	W	145	44.776	21.855	-19.009	1.00	46.18
	ATOM	4448	O	WAT	W	146	81.842	9.124	42.112	1.00	41.17

-97-

	ATOM	4449	O	WAT W 147	65.891	12.184	46.900	1.00	41.27
	ATOM	4450	O	WAT W 148	61.870	-0.694	32.618	1.00	36.54
	ATOM	4451	O	WAT W 149	53.665	-22.423	14.114	1.00	45.13
	ATOM	4452	O	WAT W 150	70.406	-11.509	9.153	1.00	39.16
5	ATOM	4453	O	WAT W 151	57.272	24.770	-5.465	1.00	53.97
	ATOM	4454	O	WAT W 152	76.932	13.052	43.714	1.00	34.28
	ATOM	4455	O	WAT W 153	46.722	-10.271	21.629	1.00	39.60
	ATOM	4456	O	WAT W 154	71.871	-14.779	14.884	1.00	41.12
	ATOM	4457	O	WAT W 155	75.221	-2.490	33.675	1.00	36.01
10	ATOM	4458	O	WAT W 156	79.538	8.216	41.312	1.00	39.15
	ATOM	4459	O	WAT W 157	37.416	-3.706	5.762	1.00	38.40
	ATOM	4460	O	WAT W 158	35.517	15.310	19.620	1.00	36.39
	ATOM	4461	O	WAT W 159	51.237	5.731	5.785	1.00	34.79
	ATOM	4462	O	WAT W 160	51.381	-1.632	26.211	1.00	44.45
15	ATOM	4463	O	WAT W 161	43.466	16.232	-32.007	1.00	52.60
	ATOM	4464	O	WAT W 162	75.662	12.257	40.222	1.00	38.37
	ATOM	4465	O	WAT W 163	32.057	-13.026	10.708	1.00	39.45
	ATOM	4466	O	WAT W 164	44.346	0.072	6.468	1.00	36.40
	ATOM	4467	O	WAT W 165	52.324	-2.560	-1.704	1.00	46.60
20	ATOM	4468	O	WAT W 166	57.861	8.649	-15.458	1.00	41.61
	ATOM	4469	O	WAT W 167	67.132	-5.044	15.257	1.00	40.23
	ATOM	4470	O	WAT W 168	59.264	-1.197	31.588	1.00	51.30
	ATOM	4471	O	WAT W 169	51.835	3.346	23.021	1.00	39.67
	ATOM	4472	O	WAT W 170	57.419	-5.177	-4.443	1.00	35.72
25	ATOM	4473	O	WAT W 171	48.627	11.775	20.770	1.00	47.02
	ATOM	4474	O	WAT W 172	64.778	-5.263	25.321	1.00	34.04
	ATOM	4475	O	WAT W 173	21.644	11.926	-2.423	1.00	35.54
	ATOM	4476	O	WAT W 174	40.345	0.581	13.671	1.00	59.11
	ATOM	4477	O	WAT W 175	65.019	-5.440	32.798	1.00	40.87
30	ATOM	4478	O	WAT W 176	44.228	-7.202	4.474	1.00	39.61
	ATOM	4479	O	WAT W 177	83.719	10.000	40.277	1.00	42.80
	ATOM	4480	O	WAT W 178	68.408	-7.591	-0.478	1.00	38.18
	ATOM	4481	O	WAT W 179	63.973	-9.992	-4.755	1.00	51.42
	ATOM	4482	O	WAT W 180	39.726	7.902	-27.189	1.00	49.92
35	ATOM	4483	O	WAT W 181	55.044	0.850	-6.811	1.00	51.09
	ATOM	4484	O	WAT W 182	25.424	1.610	-6.315	1.00	30.30
	ATOM	4485	O	WAT W 183	25.655	20.392	-3.870	1.00	43.57
	ATOM	4486	O	WAT W 184	43.760	-10.333	15.054	1.00	39.92
	ATOM	4487	O	WAT W 185	46.383	19.180	-9.597	1.00	33.30
40	ATOM	4488	O	WAT W 186	57.924	9.404	-18.120	1.00	44.22
	ATOM	4489	O	WAT W 187	58.234	-16.451	0.308	1.00	36.17
	ATOM	4490	O	WAT W 188	38.059	-19.859	11.817	1.00	32.02
	ATOM	4491	O	WAT W 189	42.349	23.603	0.069	1.00	55.22
	ATOM	4492	O	WAT W 190	62.117	0.301	41.059	1.00	47.46
45	ATOM	4493	O	WAT W 191	39.146	34.096	6.333	1.00	35.61
	ATOM	4494	O	WAT W 192	52.021	-17.641	1.723	1.00	36.52
	ATOM	4495	O	WAT W 193	30.405	15.315	-12.140	1.00	40.90
	ATOM	4496	O	WAT W 194	56.589	6.376	-25.137	1.00	50.29
	ATOM	4497	O	WAT W 195	32.292	21.747	-31.418	1.00	30.10
50	ATOM	4498	O	WAT W 196	25.932	26.262	-31.876	1.00	33.19
	ATOM	4499	O	WAT W 197	44.253	27.169	0.607	1.00	41.25
	ATOM	4500	O	WAT W 198	31.985	18.702	10.898	1.00	43.36
	ATOM	4501	O	WAT W 199	66.104	14.551	9.666	1.00	42.15
55	ATOM	4502	O	WAT W 200	65.400	14.447	48.384	1.00	54.11
	ATOM	4503	O	WAT W 201	23.164	26.745	-32.350	1.00	43.78
	ATOM	4504	O	WAT W 202	36.449	-19.529	9.775	1.00	56.52
	ATOM	4505	O	WAT W 203	37.955	9.830	-30.717	1.00	42.18
	ATOM	4506	O	WAT W 204	80.612	-6.612	30.354	1.00	58.09
	ATOM	4507	O	WAT W 205	42.193	-5.177	3.641	1.00	53.40
60	ATOM	4508	O	WAT W 206	34.846	19.253	-0.441	1.00	43.51
	ATOM	4509	O	WAT W 207	55.615	-2.982	-4.231	1.00	46.41
	ATOM	4510	O	WAT W 208	51.625	4.220	-8.519	1.00	45.10
	ATOM	4511	O	WAT W 209	25.739	8.524	-24.942	1.00	36.13
65	ATOM	4512	O	WAT W 210	68.747	17.314	21.066	1.00	43.56
	ATOM	4513	O	WAT W 211	84.666	3.989	47.339	1.00	56.35
	ATOM	4514	O	WAT W 212	39.125	28.472	0.851	1.00	43.49
	ATOM	4515	O	WAT W 213	40.758	-6.436	1.126	1.00	43.08
	ATOM	4516	O	WAT W 214	65.742	-7.673	25.260	1.00	39.84
	ATOM	4517	O	WAT W 215	68.113	-7.014	26.268	1.00	44.06
70	ATOM	4518	O	WAT W 216	50.292	24.666	-37.803	1.00	47.27
	ATOM	4519	O	WAT W 217	76.215	-4.709	32.421	1.00	35.98
	ATOM	4520	O	WAT W 218	28.732	31.945	-22.056	1.00	33.29
	ATOM	4521	O	WAT W 219	74.218	14.100	34.912	1.00	76.11
	ATOM	4522	O	WAT W 220	57.961	0.451	28.074	1.00	47.45

-98-

	ATOM	4523	O	WAT	W	221	32.590	10.932	-11.111	1.00	49.96
	ATOM	4524	O	WAT	W	222	51.203	-19.722	11.498	1.00	41.52
	ATOM	4525	O	WAT	W	223	55.448	-14.143	-4.633	1.00	36.90
5	ATOM	4526	O	WAT	W	224	21.981	23.670	-26.954	1.00	35.03
	ATOM	4527	O	WAT	W	225	38.572	-13.668	7.579	1.00	39.66
	ATOM	4528	O	WAT	W	226	56.707	-16.581	26.316	1.00	35.78
	ATOM	4529	O	WAT	W	227	70.225	2.519	46.317	1.00	45.99
	ATOM	4530	O	WAT	W	228	36.498	21.585	14.126	1.00	33.98
10	ATOM	4531	O	WAT	W	229	61.790	-13.520	-4.514	1.00	50.15
	ATOM	4532	O	WAT	W	230	64.989	-1.584	30.303	1.00	36.47
	ATOM	4533	O	WAT	W	231	38.229	27.188	10.218	1.00	45.56
	ATOM	4534	O	WAT	W	232	67.835	-7.729	5.083	1.00	34.03
	ATOM	4535	O	WAT	W	233	45.674	22.663	18.801	1.00	65.84
15	ATOM	4536	O	WAT	W	234	43.579	-5.428	17.882	1.00	43.49
	ATOM	4537	O	WAT	W	235	64.221	5.067	46.860	1.00	41.97
	ATOM	4538	O	WAT	W	236	72.469	18.804	43.000	1.00	36.08
	ATOM	4539	O	WAT	W	237	43.180	3.609	16.574	1.00	59.75
	ATOM	4540	O	WAT	W	238	34.121	16.290	-13.499	1.00	46.11
20	ATOM	4541	O	WAT	W	239	62.037	17.693	20.122	1.00	50.69
	ATOM	4542	O	WAT	W	240	37.376	10.472	-16.234	1.00	45.81
	ATOM	4543	O	WAT	W	241	26.431	22.009	-0.233	1.00	46.92
	ATOM	4544	O	WAT	W	242	25.310	12.750	-11.978	1.00	50.59
	ATOM	4545	O	WAT	W	243	19.671	9.916	-3.708	1.00	49.70
25	ATOM	4546	O	WAT	W	244	38.186	21.703	16.967	1.00	35.43
	ATOM	4547	O	WAT	W	245	40.977	-0.520	-8.992	1.00	51.53
	ATOM	4548	O	WAT	W	246	17.264	17.138	1.436	1.00	65.65
	ATOM	4549	O	WAT	W	247	59.212	-16.788	-2.401	1.00	43.21
	ATOM	4550	O	WAT	W	248	77.330	-11.434	7.852	1.00	51.89
30	ATOM	4551	O	WAT	W	249	22.908	25.131	-34.628	1.00	44.65
	ATOM	4552	O	WAT	W	250	37.272	2.059	20.950	1.00	42.62
	ATOM	4553	O	WAT	W	251	78.365	-12.406	10.087	1.00	55.28
	ATOM	4554	O	WAT	W	252	31.173	17.182	-10.252	1.00	47.60
	ATOM	4555	O	WAT	W	253	48.516	-12.376	-1.883	1.00	33.36
35	ATOM	4556	O	WAT	W	254	43.940	18.919	-6.022	1.00	54.48
	ATOM	4557	O	WAT	W	255	30.610	3.062	18.104	1.00	46.62
	ATOM	4558	O	WAT	W	256	72.364	2.032	11.881	1.00	60.78
	ATOM	4559	O	WAT	W	257	36.491	-6.172	6.630	1.00	48.36
	ATOM	4560	O	WAT	W	258	65.789	-10.191	31.731	1.00	42.15
40	ATOM	4561	O	WAT	W	259	59.438	15.957	21.720	1.00	40.75
	ATOM	4562	O	WAT	W	260	31.766	20.345	7.940	1.00	41.46
	ATOM	4563	O	WAT	W	261	38.175	22.668	9.740	1.00	36.51
	ATOM	4564	O	WAT	W	262	69.731	20.766	38.855	1.00	45.16
	ATOM	4565	O	WAT	W	263	25.834	32.385	-27.930	1.00	39.41
45	ATOM	4566	O	WAT	W	264	70.140	-4.383	3.316	1.00	42.01
	ATOM	4567	O	WAT	W	265	17.686	28.637	-27.597	1.00	36.50
	ATOM	4568	O	WAT	W	266	30.498	10.397	17.979	1.00	38.49
	ATOM	4569	O	WAT	W	267	41.552	17.448	-14.793	1.00	45.70
	ATOM	4570	O	WAT	W	268	43.965	-4.267	15.684	1.00	47.33
50	ATOM	4571	O	WAT	W	269	24.247	23.631	-0.377	1.00	52.61
	ATOM	4572	O	WAT	W	270	39.439	16.949	-2.045	1.00	40.49
	ATOM	4573	O	WAT	W	271	49.374	23.294	3.413	1.00	46.56
	ATOM	4574	O	WAT	W	272	39.872	8.421	-18.197	1.00	45.41
	ATOM	4575	O	WAT	W	273	46.466	-1.275	7.239	1.00	47.88
55	ATOM	4576	O	WAT	W	274	29.019	38.205	-20.300	1.00	61.46
	ATOM	4577	O	WAT	W	275	69.375	1.409	13.444	1.00	43.48
	ATOM	4578	O	WAT	W	276	72.207	3.732	29.386	1.00	40.43
	ATOM	4579	O	WAT	W	277	39.712	37.170	0.051	1.00	39.08
	ATOM	4580	O	WAT	W	278	48.094	-1.929	10.639	1.00	35.23
60	ATOM	4581	O	WAT	W	279	46.176	-0.007	10.070	1.00	57.82
	ATOM	4582	O	WAT	W	280	34.060	14.226	-7.694	1.00	47.69
	ATOM	4583	O	WAT	W	281	66.985	-1.458	15.223	1.00	40.31
	ATOM	4584	O	WAT	W	282	69.909	-11.226	6.382	1.00	54.99
	ATOM	4585	O	WAT	W	283	27.681	22.895	8.733	1.00	41.91
65	ATOM	4586	O	WAT	W	284	44.274	-3.092	9.331	1.00	47.80
	ATOM	4587	O	WAT	W	285	35.726	14.777	-5.459	1.00	63.96
	ATOM	4588	O	WAT	W	286	36.355	13.676	-2.214	1.00	51.47
	ATOM	4589	O	WAT	W	287	45.262	7.207	17.415	1.00	54.68
	ATOM	4590	O	WAT	W	288	68.185	20.756	43.230	1.00	51.92
70	ATOM	4591	O	WAT	W	289	61.045	16.189	10.892	1.00	47.39
	ATOM	4592	O	WAT	W	290	37.948	29.641	-14.217	1.00	51.54
	ATOM	4593	O	WAT	W	291	25.752	1.732	16.571	1.00	50.52
	ATOM	4594	O	WAT	W	292	21.651	4.509	5.878	1.00	55.37
	ATOM	4595	O	WAT	W	293	57.826	3.992	44.663	1.00	46.21
	ATOM	4596	O	WAT	W	294	66.103	19.731	40.130	1.00	39.58

-99-

	ATOM	4597	O	WAT	W	295	46.479	-4.707	17.542	1.00	44.15
	ATOM	4598	O	WAT	W	296	71.219	-3.422	0.474	1.00	42.17
	ATOM	4599	O	WAT	W	297	39.881	2.904	14.591	1.00	39.80
5	ATOM	4600	O	WAT	W	298	56.543	16.797	18.584	1.00	46.72
	ATOM	4601	O	WAT	W	299	61.789	-18.999	2.206	1.00	57.02
	ATOM	4602	O	WAT	W	300	42.705	10.878	-13.312	1.00	41.71
	ATOM	4603	O	WAT	W	301	69.432	7.509	6.399	1.00	56.46
	ATOM	4604	O	WAT	W	302	50.399	1.771	-8.208	1.00	46.36
	ATOM	4605	O	WAT	W	303	80.707	8.597	32.436	1.00	57.84
10	ATOM	4606	O	WAT	W	304	35.950	-3.190	-6.617	1.00	47.01
	ATOM	4607	O	WAT	W	305	63.191	13.663	10.338	1.00	47.69
	ATOM	4608	O	WAT	W	306	32.746	17.045	16.882	1.00	38.37
	ATOM	4609	O	WAT	W	307	55.795	22.081	-3.121	1.00	45.39
	ATOM	4610	O	WAT	W	308	52.917	-15.266	-5.084	1.00	58.04
15	ATOM	4611	O	WAT	W	309	32.990	20.281	-2.705	1.00	41.15
	ATOM	4612	O	WAT	W	310	65.221	-0.521	13.373	1.00	50.04
	ATOM	4613	O	WAT	W	311	31.445	8.146	-16.640	1.00	47.12
	ATOM	4614	O	WAT	W	312	70.526	-1.084	-1.047	1.00	43.90
	ATOM	4615	O	WAT	W	313	67.588	-6.363	21.900	1.00	57.15
20	ATOM	4616	O	WAT	W	314	66.096	-4.686	20.242	1.00	69.24
	ATOM	4617	O	WAT	W	315	47.292	23.337	13.967	1.00	42.45
	ATOM	4618	O	WAT	W	316	77.697	-6.690	46.864	1.00	61.61
	ATOM	4619	O	WAT	W	317	57.134	18.189	-19.802	1.00	61.48
	ATOM	4620	O	WAT	W	318	56.615	6.099	-16.259	1.00	55.28
25	ATOM	4621	O	WAT	W	319	70.759	17.127	50.284	1.00	46.60
	ATOM	4622	O	WAT	W	320	72.021	-17.283	5.694	1.00	53.07
	ATOM	4623	O	WAT	W	321	23.729	4.269	-4.449	1.00	58.06
	ATOM	4624	O	WAT	W	322	22.138	20.117	-24.492	1.00	37.83
	ATOM	4625	O	WAT	W	323	40.526	13.448	-0.063	1.00	54.95
30	ATOM	4626	O	WAT	W	324	28.034	-4.586	23.421	1.00	50.98
	ATOM	4627	O	WAT	W	325	38.920	16.623	-33.391	1.00	53.48
	ATOM	4628	O	WAT	W	326	77.040	-7.476	27.616	1.00	73.56
	ATOM	4629	O	WAT	W	327	68.678	-0.075	28.998	1.00	51.90
	ATOM	4630	O	WAT	W	328	46.505	7.743	-11.664	1.00	43.38
35	ATOM	4631	O	WAT	W	329	43.657	18.299	-3.514	1.00	20.00
	ATOM	4632	O	WAT	W	330	40.596	13.269	-4.354	1.00	20.00
	ATOM	4633	O	WAT	W	331	66.428	-1.404	17.847	1.00	20.00
	ATOM	4634	O	WAT	W	332	41.584	19.897	-1.703	1.00	20.00
	ATOM	4635	O	WAT	W	333	41.694	22.971	-4.274	1.00	20.00
40	ATOM	4636	O	WAT	W	334	67.997	3.764	15.541	1.00	20.00
	ATOM	4637	O	WAT	W	335	60.537	18.286	2.068	1.00	20.00
	ATOM	4638	O	WAT	W	336	56.447	20.428	10.716	1.00	20.00
	ATOM	4639	O	WAT	W	337	55.557	22.546	9.246	1.00	20.00
	ATOM	4640	O	WAT	W	338	58.179	16.183	-0.749	1.00	20.00
45	ATOM	4641	O	WAT	W	339	58.887	16.112	-3.916	1.00	20.00
	ATOM	4642	O	WAT	W	340	63.509	11.351	2.806	1.00	20.00
	ATOM	4643	O	WAT	W	341	62.716	14.296	1.151	1.00	20.00
	ATOM	4644	O	WAT	W	342	39.563	-4.272	12.971	1.00	20.00
	ATOM	4645	O	WAT	W	343	39.743	-6.346	11.592	1.00	20.00
50	ATOM	4646	O	WAT	W	344	44.345	-8.782	9.282	1.00	20.00
	ATOM	4647	O	WAT	W	345	38.126	-6.949	4.925	1.00	20.00
	ATOM	4648	O	WAT	W	346	41.558	-9.568	2.423	1.00	20.00
	ATOM	4649	O	WAT	W	347	46.133	-8.864	-1.132	1.00	20.00
	ATOM	4650	O	WAT	W	348	42.431	12.582	19.513	1.00	20.00
55	ATOM	4651	O	WAT	W	349	39.817	3.709	21.589	1.00	20.00
	ATOM	4652	O	WAT	W	350	40.535	5.544	20.119	1.00	20.00
	ATOM	4653	O	WAT	W	351	41.467	8.090	20.981	1.00	20.00
	ATOM	4654	O	WAT	W	352	61.469	16.879	-5.628	1.00	20.00
	ATOM	4655	O	WAT	W	353	57.522	13.280	-9.676	1.00	20.00
60	ATOM	4656	O	WAT	W	354	57.275	9.042	-5.426	1.00	20.00
	ATOM	4657	O	WAT	W	355	59.327	5.417	-6.085	1.00	20.00
	ATOM	4658	O	WAT	W	356	52.962	-4.323	-3.179	1.00	20.00
	ATOM	4659	O	WAT	W	357	36.344	-8.909	7.979	1.00	20.00
	ATOM	4660	O	WAT	W	358	42.391	30.320	-15.418	1.00	20.00
65	ATOM	4661	O	WAT	W	359	52.354	18.876	-21.657	1.00	20.00
	ATOM	4662	O	WAT	W	360	85.510	2.059	39.934	1.00	20.00
	ATOM	4663	O	WAT	W	361	86.895	4.068	37.822	1.00	20.00
	ATOM	4664	O	WAT	W	362	81.610	8.015	30.106	1.00	20.00
	ATOM	4665	O	WAT	W	363	81.600	7.773	49.392	1.00	20.00
70	ATOM	4666	O	WAT	W	364	76.414	9.988	52.505	1.00	20.00
	ATOM	4667	O	WAT	W	365	67.897	8.778	49.346	1.00	20.00
	ATOM	4668	O	WAT	W	366	63.858	2.436	46.800	1.00	20.00
	ATOM	4669	O	WAT	W	367	71.953	1.096	48.138	1.00	20.00
	ATOM	4670	O	WAT	W	368	89.873	-11.648	35.808	1.00	20.00

-100-

	ATOM	4671	O	WAT W 369	88.460	-12.813	38.004	1.00	20.00
	ATOM	4672	O	WAT W 370	91.761	-9.669	35.928	1.00	20.00
	ATOM	4673	O	WAT W 371	88.580	-15.367	38.475	1.00	20.00
5	ATOM	4674	O	WAT W 372	76.861	-9.543	44.348	1.00	20.00
	ATOM	4675	O	WAT W 373	74.471	-6.743	45.210	1.00	20.00
	ATOM	4676	O	WAT W 374	79.402	-2.424	46.754	1.00	20.00
	ATOM	4677	O	WAT W 375	75.647	-0.122	49.778	1.00	20.00
	ATOM	4678	O	WAT W 376	77.752	1.584	49.411	1.00	20.00
10	ATOM	4679	O	WAT W 377	37.468	-4.589	21.373	1.00	20.00
	ATOM	4680	O	WAT W 378	45.334	-7.735	21.716	1.00	20.00
	ATOM	4681	O	WAT W 379	46.136	-5.299	22.588	1.00	20.00
	ATOM	4682	O	WAT W 380	43.144	-7.232	20.423	1.00	20.00
	ATOM	4683	O	WAT W 381	42.129	-4.775	20.988	1.00	20.00
15	ATOM	4684	O	WAT W 382	47.659	-14.000	24.499	1.00	20.00
	ATOM	4685	O	WAT W 383	41.892	-6.834	15.632	1.00	20.00
	ATOM	4686	O	WAT W 384	42.961	-8.398	13.868	1.00	20.00

-101-

Table 2

Composition of defined minimal culture medium for selenium-containing PS. All components were filter-sterilized through 0.22µm filters, except where indicated.

Compound	Stock conc.	Volume	Comments
M9 medium ^a	1	250 ml	Autoclaved.
MgSO ₄	1 M	250 µl	Autoclaved separately from M9 medium to avoid precipitation.
D-glucose	4% w/v	25 ml	Not autoclaved, since that caused glucose to caramelize (yellow colour); filter sterilized instead.
Thiamine	0.5% w/v	25 µl	Prepared stock and stored at -20°C; since repeated cycles of freeze and thaw do not damage it.
FeSO ₄	4.2 g/l	250 µl	Prepared stock and stored at -20°C, to prevent oxidation.
Ampicillin	100 mg/ml	250 µl	Filter sterilized and stored as aliquots – cycles of freeze and thaw were avoided.
IPTG	70 mg/ml	250 µl	
L-arginine	2.53% w/v	5 ml	Supplemented for AT1371 deficiency; prepared together as single stock.
L-histidine	0.31% w/v		
L-proline	4.6% w/v		
Adenine	1.35% w/v		
L-lysine	12.5 g/l	2 ml	Cocktail for methionine pathway inhibition; prepared as one stock. Final concentrations were 100 and 50 mg/l respectively.
L-phenylalanine	12.5 g/l		
L-threonine	12.5 g/l		
L-isoleucine	6.25 g/l		
L-leucine	6.25 g/l		
L-valine	6.25 g/l		
L-seleno-methionine	Final conc: 50 mg/l	-	No need to sterilise, to minimise risk of oxidation. Dissolved in water directly in bottle in which supplied, then added.

^a Sambrook, J., Fritsch, E. F. & Maniatis, T. (1989). *Molecular cloning: a laboratory manual*, 2nd ed. Cold Spring Harbour Laboratory Press, Cold Spring Harbor, N.Y.

Table 3

<i>Crystallographic refinement</i>		
No. reflexions (test set)	77 294 (4062)	Test set is excluded from refinement for cross-validation
No. restraints	15 730	Restraints in TNT with a weight assigned
No. parameters	20 236	
Weight for geom. restraints (TNT)	3	
<i>Final model parameters</i>		
Residues	566	
Hetero	1 Tris, 2 ethanediol	
No. water molecules	622	
No. non-hydrogen atoms	5059	
Resolution range (Å)	45 - 1.7	
<i>Refinement convergence</i>		
R_{free}	24.9	R_{factor} calculated using test reflexions
R_{factor}	22.6	$R_{factor} = \sum_h F_{obs} - F_{calc} / \sum_h F_{obs} $, w/o test reflexions.
DDQ (score, ranking)	UFO	"Unassigned positive Feature left-Over score"
	DDQ-R	Ratio of Shift and Water peak contributions.
Average B-factor, subunit A (Å ²)	33.9	
subunit B (Å ²)	36.4	
waters (Å ²)	47.8	
Wilson distribution B_{factor} (Å ²)	28.0	
<i>Model quality</i>		
Ramachandran plot	% residues in most favoured region	92.2
	% residues in generously-allowed region	7.4
	No. residues in disallowed region	0
Rms deviation from ideal ("root mean square")	Covalent bond lengths (Å)	0.018
	Bond angles (°)	1.41
	Planar groups (Å)	0.007
Procheck criteria	% bond lengths outside expected limits	2.6
	% bond angles outside expected limits	3.1
	% planar groups outside expected limits	1.0
WhatCheck criteria	No. unsaturated H-bonds	2
	No. residues in unusual environments	14

-103-

Table 4

Residues lining the PS binding pockets

5	Val27
	Pro28
	Thr29
	Met30
	Gly31
10	Asn32
	Leu33
	His34
	Asp35
	Gly36
15	His37
	Lys39
	Leu40
	Ser54
	Phe56
20	Asn58
	Gln61
	Phe62
	Tyr71
	Phe91
25	Pro93
	Ile98
	Leu118
	Glu119
	His126
30	Phe127
	Val130
	Ile133
	Val134
	Lys136
35	Leu137
	Leu140
	Cys147
	Phe148
	Gly149
40	Glu150
	Lys151
	Asp152
	Phe153
	Gln154
45	Gln155
	Leu156
	Ile159
	Ile172
	Val175
50	Pro176
	Ile177
	Met178
	Arg179
	Leu184
55	Ala185
	Leu186
	Ser187
	Ser188
	Arg189
60	Asn190
	Asp242
	Leu251
	Leu264
	Val265
65	Ala266
	Arg273
	Leu274
	Ile275
	Asp276
70	Asn277

Claims:

1. A crystal of pantothenate synthetase (PS) having a monoclinic space group $P2_1$ and unit cell dimensions of $a = 66.0 \pm 0.2 \text{ \AA}$, $b = 78.1 \pm 0.2 \text{ \AA}$, $c = 77.1 \pm 0.2 \text{ \AA}$ and $\beta = 103.7 \pm 0.2^\circ$.
2. A crystal of PS having the three dimensional atomic coordinates of Table 1.
3. A method for crystallizing a selenium atom PS derivative which comprises producing PS by recombinant production in a bacterial host in the presence of selenomethionine, recovering a selenium atom PS derivative from the host and growing crystals from the recovered selenium atom PS derivative.
4. A computer-based method of rational drug design which comprises:
 - providing the structure of the PS as defined by the coordinates of Table 1;
 - providing the structure of a candidate modulator molecule; and
 - fitting the structure of the candidate modulator molecule to the structure of the PS of Table 1.
5. A computer-based method of rational drug design which comprises:
 - providing the coordinates of at least two atoms of the PS of Table 1;
 - providing the structure of a candidate modulator molecule; and
 - fitting the structure of the candidate modulator molecule to the provided coordinates of the PS.
6. A computer-based method of rational drug design which comprises:

-105-

providing the coordinates of at least a sub-domain of the
PS;

providing the structure of a candidate modulator molecule;
and

5 fitting the structure of the candidate modulator molecule
to the coordinates of the PS sub-domain provided.

7. The method of any one of claims 4 to 6 which further
comprises the steps of:

10 obtaining or synthesising the candidate modulator; and
contacting the candidate modulator with PS to determine
the ability of the candidate modulator to interact with PS.

8. The method of any one of claims 4 to 6 which further
15 comprises the steps of:

obtaining or synthesising said candidate modulator;
forming a complex of PS and said potential modulator; and
analysing said complex by X-ray crystallography to
determine the ability of said candidate modulator to interact
20 with PS.

9. A compound having a chemical structure selected using the
method of any one of claims 4 to 6, said compound being an
inhibitor of PS.

25 10. A computer readable medium with either (a) atomic data
according to Table 1 recorded thereon, said data defining the
three-dimensional structure of PS or at least one sub-domain
thereof or (b) structure factor data for PS recorded thereon,
30 the structure factor data being derivable from the atomic
coordinate data of Table 1.

11. A computer system, intended to generate structures and/or
perform rational drug design for PS or complexes of PS with a

-106-

- potential modulator, the system containing either (a) atomic coordinate data according to Table 1, said data defining the three-dimensional structure of PS or at least one sub-domain thereof or (b) structure factor data for PS, said structure factor data being derivable from the atomic coordinate data of Table 1.
- 5

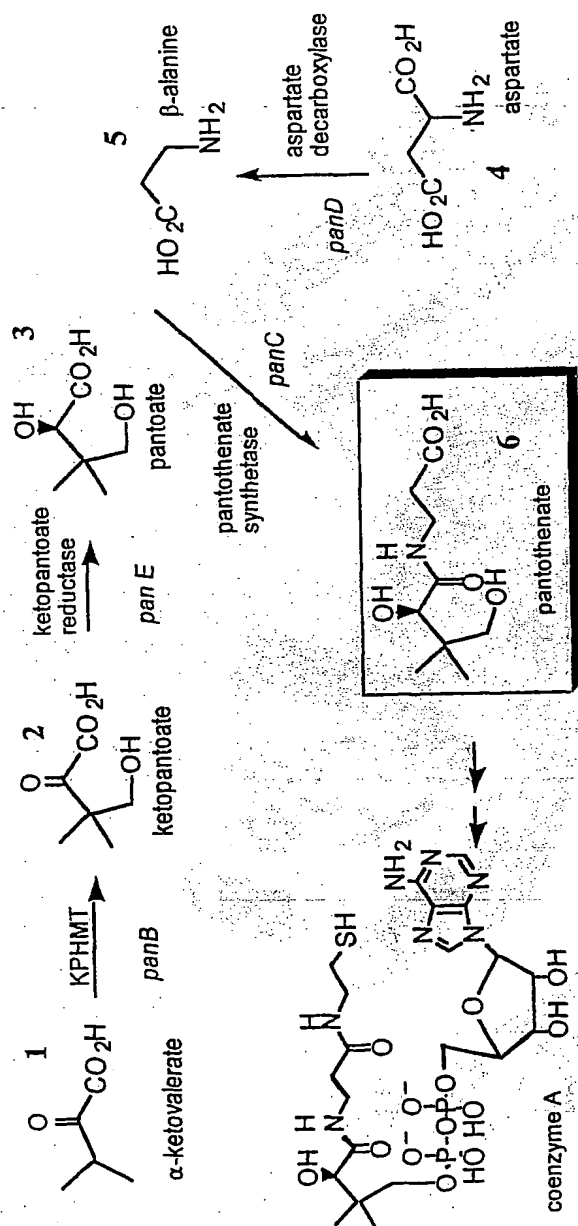


Fig. 1



Fig. 2a

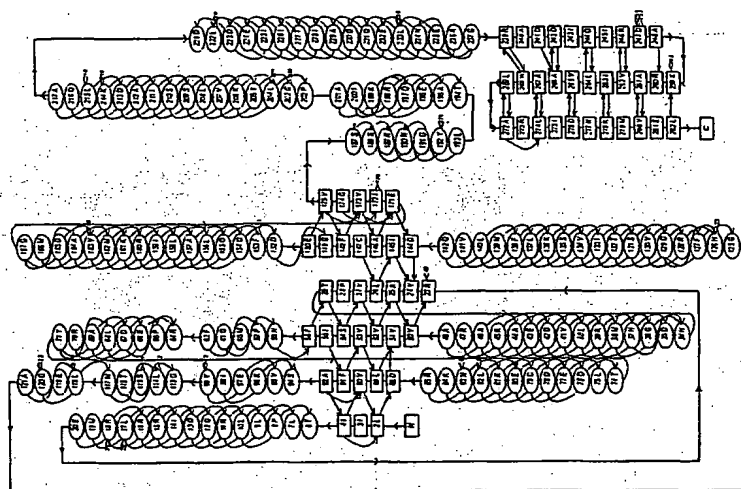


Fig. 2c

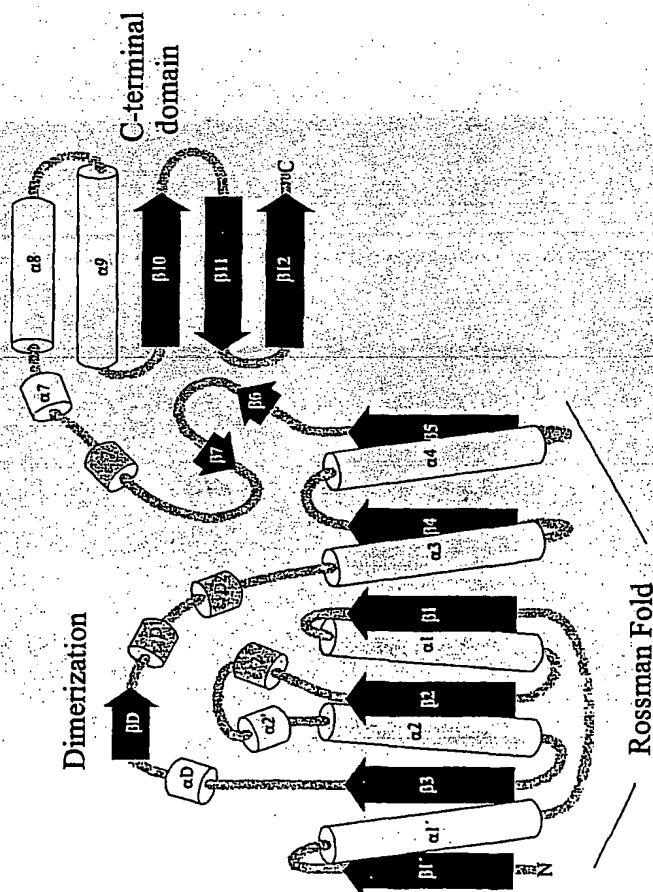


Fig. 2b

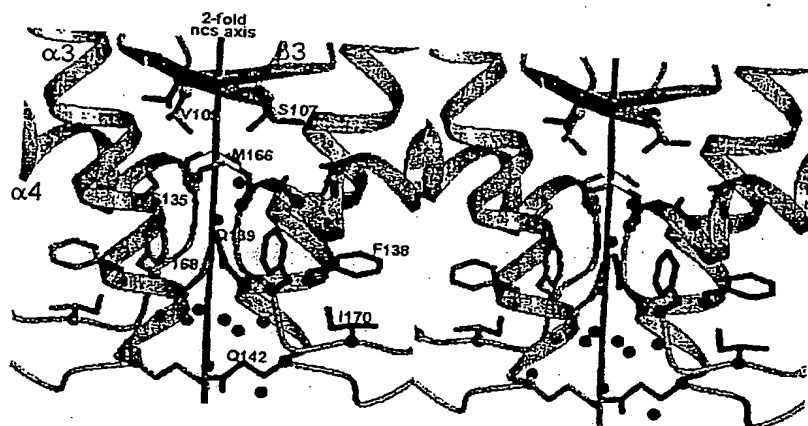


Fig. 3

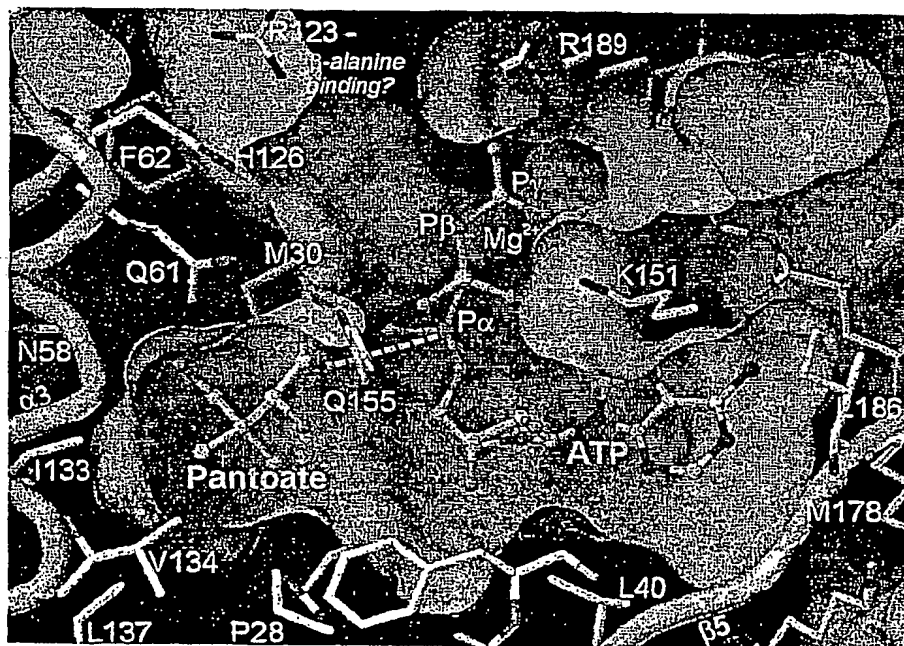


Fig. 4

INTERNATIONAL SEARCH REPORT

Int. Application No

PCT/GB 01/04067

A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 C12N9/00 G06F17/50

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 C12N G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, BIOSIS, WPI Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P, X	<p>DELFT ET AL: "The crystal structure of E. coli pantothenate synthetase confirms it as a member of the cytidyltransferase superfamily"</p> <p>STRUCTURE ,</p> <p>vol. 9, May 2001 (2001-05), pages 439-450, XP002187263</p> <p>* See page 441 (Table 1), page 442 (Figure 2), page 448 (Experimental Procedures) and page 450 (footnote -> PDB = 1IH0; release date: 30.05.2001 *</p> <p style="text-align: center;">-/-</p>	1-8, 10, 11

☒ Further documents are listed in the continuation of box C.☐ Patent family members are listed in annex.

* Special categories of cited documents :

- *A* document defining the general state of the art which is not considered to be of particular relevance
- *E* earlier document but published on or after the international filing date
- *L* document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- *O* document referring to an oral disclosure, use, exhibition or other means
- *P* document published prior to the international filing date but later than the priority date claimed

T later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

X document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

Y document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

* & * document member of the same patent family

Date of the actual completion of the international search

14 January 2002

Date of mailing of the international search report

04/02/2002

Name and mailing address of the ISA

European Patent Office, P.B. 5818 Patentlaan 2
 NL - 2280 HV Rijswijk
 Tel. (+31-70) 340-2040, Tx. 31 651 epo nl,
 Fax: (+31-70) 340-3016

Authorized officer

Korsner, S-E

INTERNATIONAL SEARCH REPORT

Int. Application No

PCT/GB 01/04067

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	<p>QORONFLEH ET AL: "Production of selenomethionine-labeled recombinant human neutrophil collagenase in Escherichia coli"</p> <p>JOURNAL OF BIOTECHNOLOGY, ELSEVIER SCIENCE PUBLISHERS, AMSTERDAM, NL, vol. 39, no. 2, 15 April 1995 (1995-04-15), pages 119-128, XP004036977</p> <p>ISSN: 0168-1656</p> <p>* See pages 119-120</p> <p>(Introduction/Selenomethionine/MAD) *</p>	1-8,10, 11
A	<p>SHAO ET AL: "Accessibility of selenomethionine proteins by total chemical synthesis: structural studies of human herpesvirus-8 MIP-II"</p> <p>FEBS LETTERS, ELSEVIER SCIENCE PUBLISHERS, AMSTERDAM, NL, vol. 441, no. 1, 11 December 1998 (1998-12-11), pages 77-82, XP004258875</p> <p>ISSN: 0014-5793</p> <p>* See page 77 (Introduction) *</p>	1-8,10, 11
T	<p>JHOTI H: "High-throughput structural proteomics using x-rays"</p> <p>TRENDS IN BIOTECHNOLOGY, ELSEVIER PUBLICATIONS, CAMBRIDGE, GB, vol. 19, no. 10, 1 October 2001 (2001-10-01), pages S67-S71, XP004310381</p> <p>ISSN: 0167-7799</p> <p>* See pages S69-S70 (Structure to drug lead) *</p>	1-8,10, 11

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Claims Nos.: 9

Present Claim 9 relates to undefined compounds that may be obtained by using the method of Claims 4-6. This is merely a desideratum, and no such compounds have been identified by the Applicant. Since they are undefined, it is not possible to carry out a meaningful search.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.